
Deep Learning Meets Double Machine Learning: Causal Inference with Large-Scale Combinatorial Experiments

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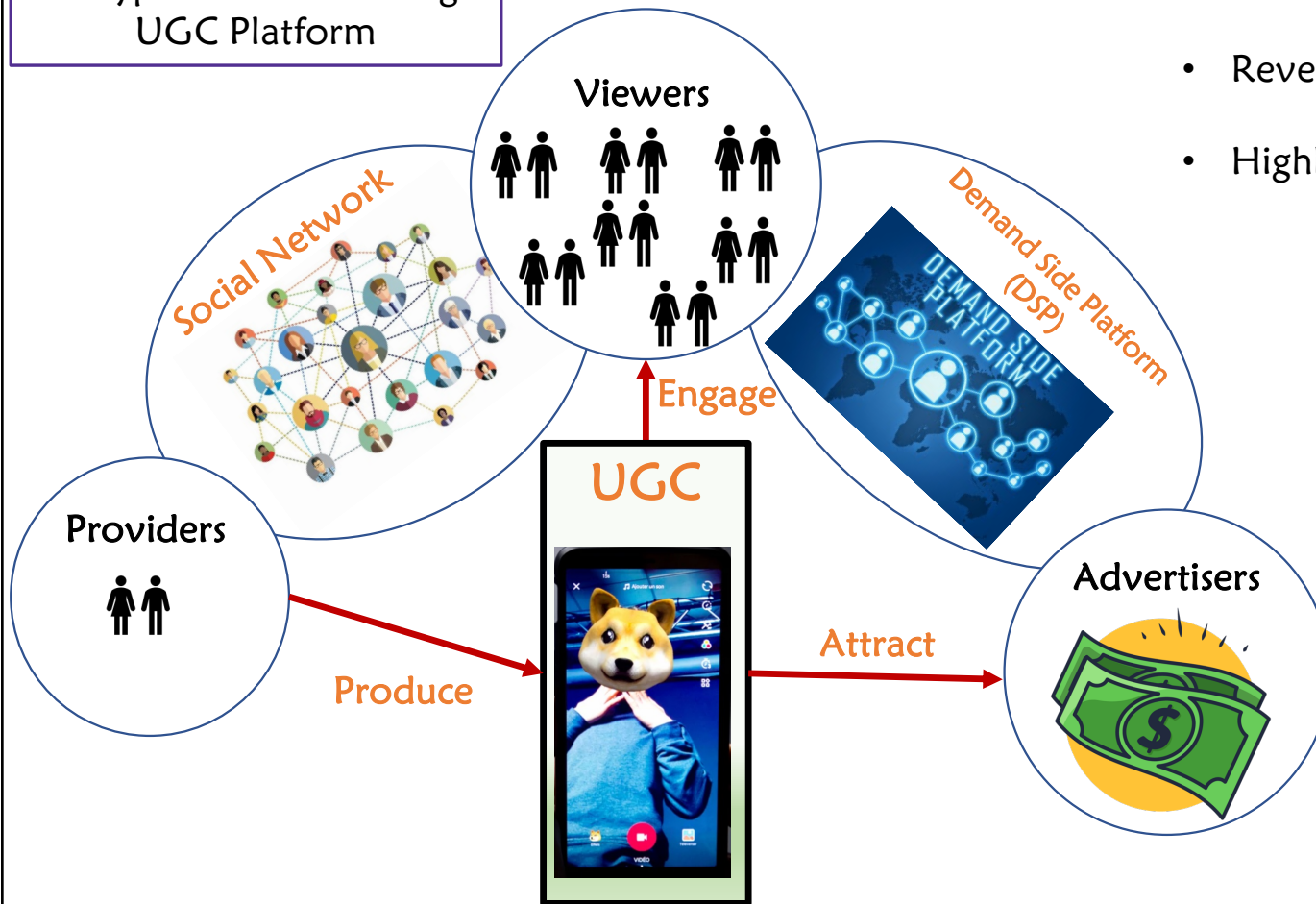
(Based on the joint work with Zikun Ye, Zhiqi Zhang, Dennis J. Zhang, Heng Zhang)

1. Introduction

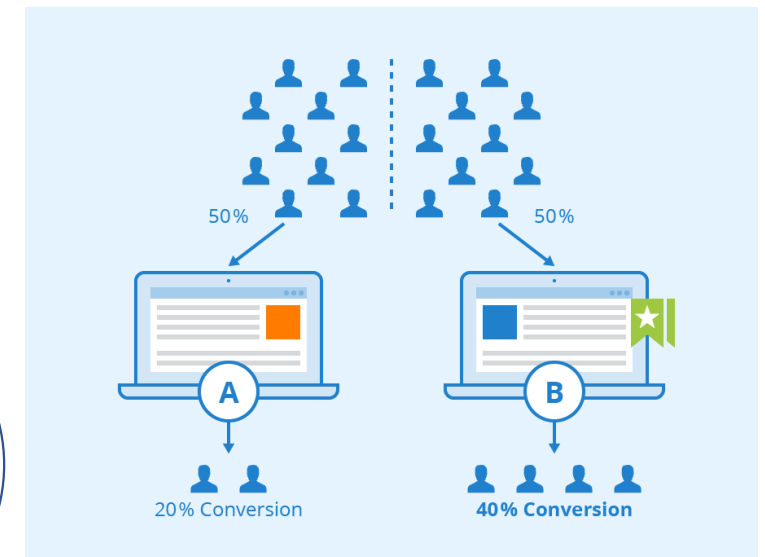
2. Theory: Deep Learning, Double Machine Learning, and Asymptotics
3. Empirics: Implementation, Experiments, and Validations with Real and Synthetic Data

Video-Sharing UGC Platforms and A/B Tests

A Typical Video-Sharing UGC Platform

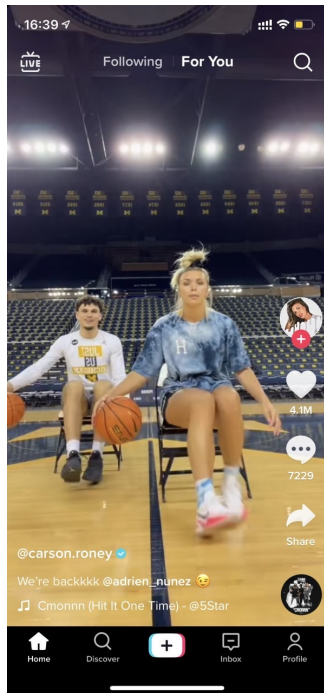


- MAU in **billions** (53.6% of world population).
- Revenue in **hundreds of billions of USD** per year.
- Highly **individualized big data**.

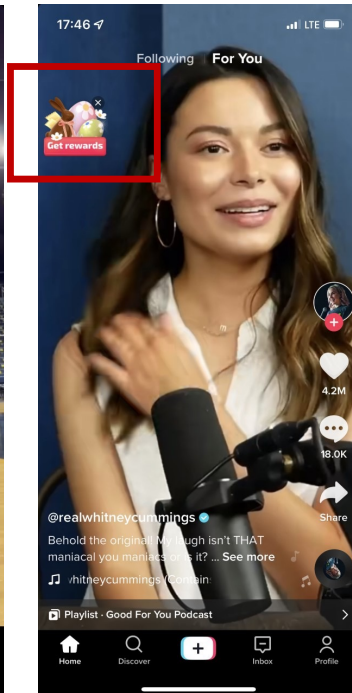


A/B Testing: The Decision Engine

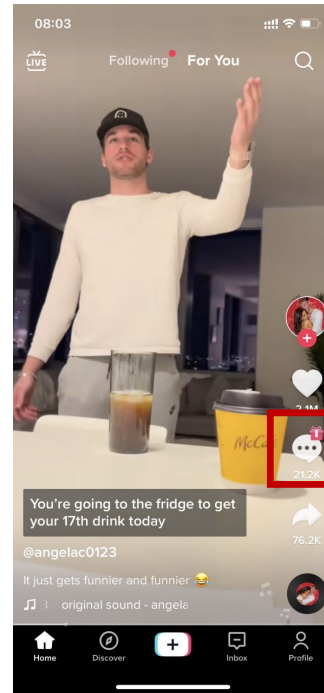
Multiple A/B Tests on Large-Scale Platforms



Baseline: Nothing



Treatment A:
“Get Rewards”



Treatment B:
“Send Gift”

- A large-scale platform launches **hundreds of A/B tests everyday** to fast iterate their operations and marketing strategies.
 - Usually under the **orthogonal design**.
- Users are independently treated by thousands of different A/B tests **simultaneously**.

How to estimate and infer the **combined treatment effect** of **multiple A/B tests**?

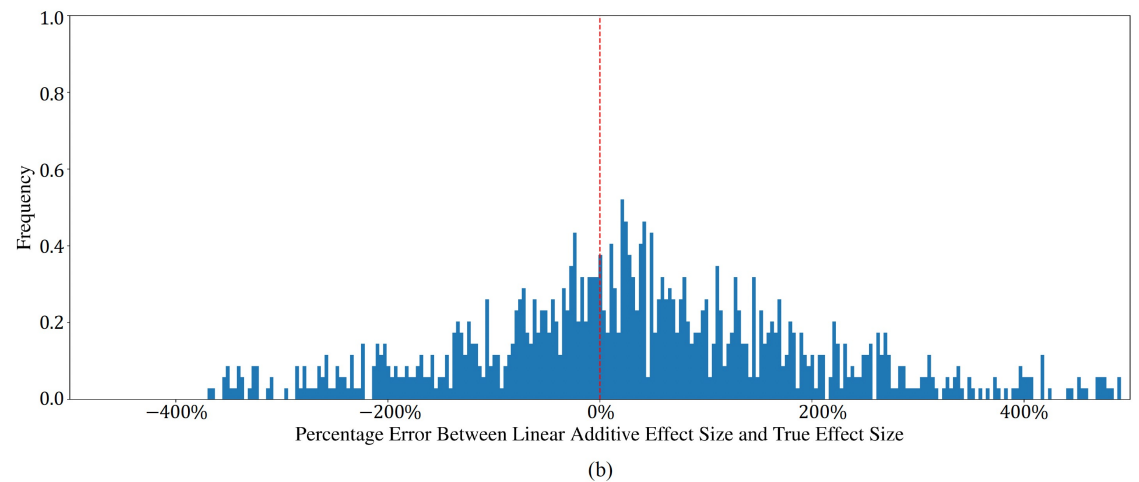
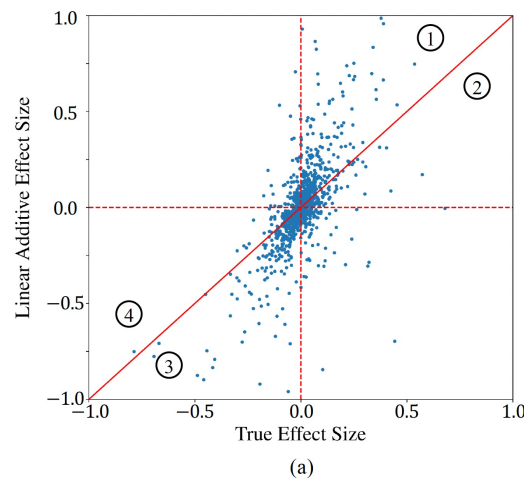
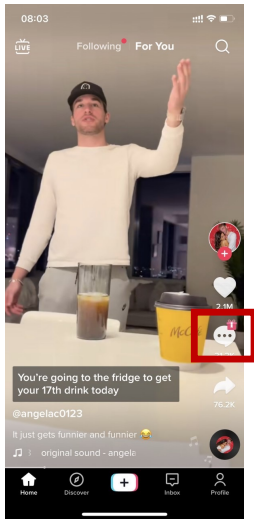
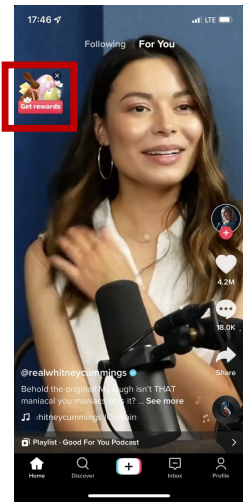
Solution 1: Linear Addition

- Effect of “Get Rewards + Send Gift” = Effect of “Get Rewards” + Effect of “Send Gift”

Control	Treatment A	Treatment B
No button	Get Rewards	Send Gift

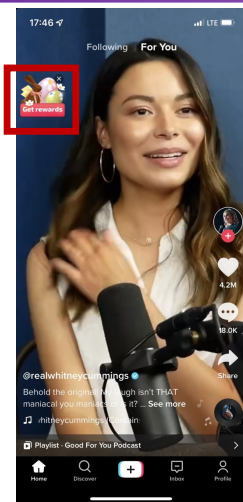
Limitations:

- Non-linearity:** The effect of the combined treatment may not equal the sum of each.
 - Decreasing marginal return:** (+7min) < (+3min) + (+5min)
 - Increasing marginal return:** (+15min) > (+6min) + (+7min)



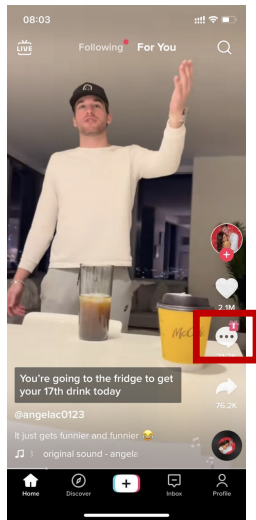
- Heterogeneity:** The effect of the combined treatment may vary for different users.

Solution 2: Factorial Experiment



- Run an experiment with treatment combinations “Get Rewards” , “Send Gift” and “Get Rewards + Send Gift” .

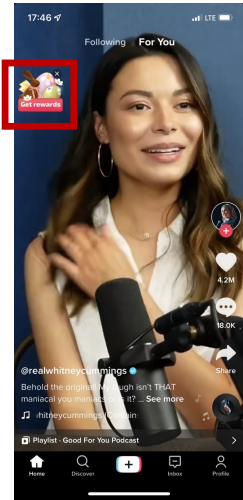
Control	Treatment A	Treatment B	Treatment AB
No button	Get Rewards	Send Gift	Get Rewards and Send Gift



Limitation:

- m interventions generate 2^m treatment combinations.
- It is impossible to even assign **only 1 user** to each single treatment combination if $m > 30$.

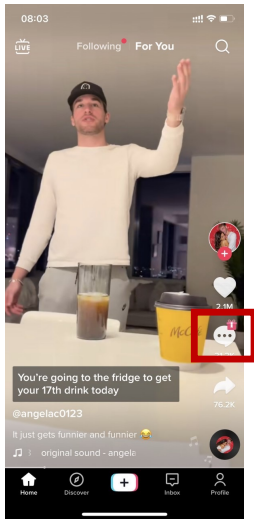
Solution 3: End-to-End Deep Learning



- Directly predict the outcome of each user under each treatment combination using **end-to-end (e2e) deep learning (DL)**.

Control	Treatment A	Treatment B
No button	Get Rewards	Send Gift

Limitations:

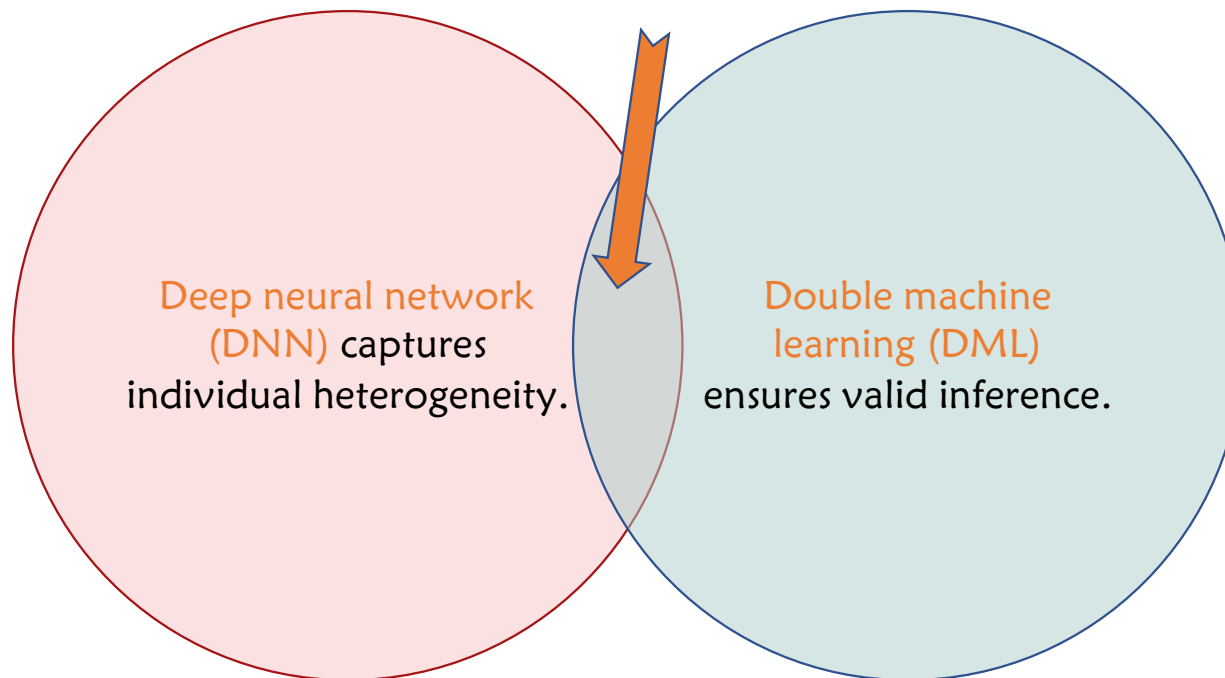


- With **unobserved treatment combinations**, we **cannot do causal inference** with e2e DL (or any other **pure machine learning** methods such as **uplift modeling**).
 - Hard to obtain any economic and managerial insights.
- How about the generalized random (causal) forests (Athey et al. 2019)?
 - Given the **unobservable** treatment combinations, causal trees/forests are essentially **(locally) linear**.

Key Research (and Business) Questions

Only observing the outcomes of a **subset of treatment combinations**:

- How to estimate and infer the **effect of any treatment combination (i.e., ATE) under multiple A/B tests** on the platform?
- How to identify the **optimal treatment combination (i.e., best-arm identification)**?



Related Literature



- **Double/de-biased machine learning (DML):** Correct the bias of a plug-in estimator through **Neyman-orthogonal score functions**.
 - Newey (1994), Chernozhukov et al. (2018, 2022), Farrell et al. (2020, 2021), Athey et al. (2018), Ellickson et al. (2022), Fan et al. (2022), etc.
- **Valid estimation and inference under experimentation:** Variance reduction and de-biasing.
 - Azevedo et al. (2020), Dasgupta et al. (2015), Athey et al. (2021), Johari et al. (2021), Bojinov et al. (2021), Candogan et al. (2021), Xiong et al. (2022), etc.
- **Experiments on online platforms:** Evaluating and optimizing the strategies of a large-scale online platform.
 - Ye et al. (2022), Zeng et al. (2022), Zhang et al. (2020), Cui et al. (2019, 2020), Feldman et al. (2021), Schwartz et al. (2017), etc.

Highlight of Main Contributions

- Theory

- A new DL+DML framework.
- Theoretical validity (consistency and normality) via Neyman orthogonality.



- Empirics

- Implementation for real large-scale A/B tests on a video-sharing platform.
- Better performance than the linear and DL benchmarks in ATE estimation and best-arm identification.

- Practice

- Practical validations of DL+DML with data from large-scale field experiments ($N > 2,000,000$).
- Inspirations for future researchers and practitioners to apply DL+DML.

1. Introduction
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Deep Learning Framework: Setup

- The platform runs m A/B tests, each with a binary treatment. Use $\mathbf{t} \in \{0,1\}^m$ to denote a treatment combination.
 - For example, $m = 4, \mathbf{t} = (0, 0, 1, 0)'$ represents that the user is in the control condition of A/B test A, B, and D, and in the treatment condition of A/B test C.

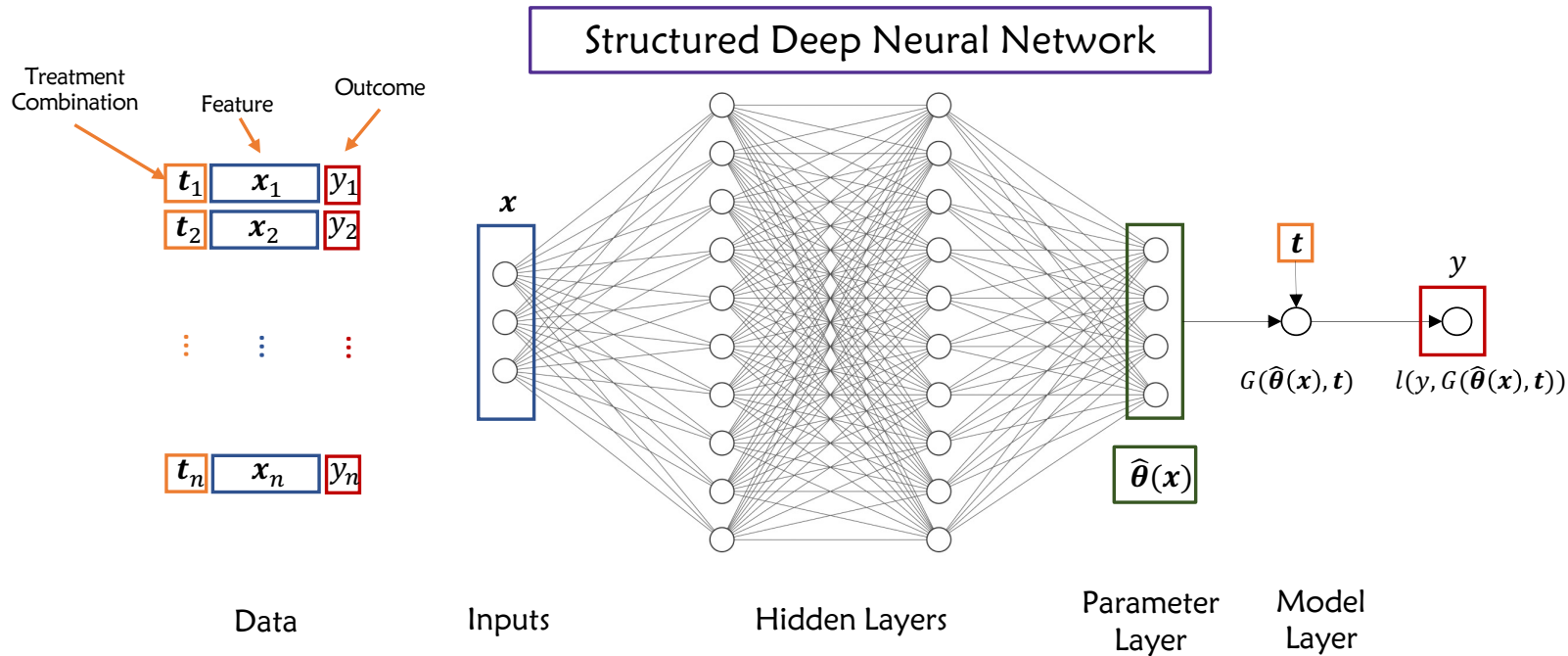
- Outcome $Y \in \mathbb{R}$ and feature $\mathbf{X} \in \mathbb{R}^{d_x}$.

- Assume the data generating process (DGP):

$$\mathbb{E}[Y|\mathbf{X} = \mathbf{x}, \mathbf{T} = \mathbf{t}] = G(\boldsymbol{\theta}^*(\mathbf{x}), \mathbf{t})$$

- $G(\boldsymbol{\theta}, \mathbf{t})$ is the link function with a known (parametric) structure, mapping $\mathbb{R}^{d_x} \times \{0,1\}^m \rightarrow \mathbb{R}$
- $\boldsymbol{\theta}^*(\cdot)$ is the (true) nonparametric function capturing HTE and obtained by $\boldsymbol{\theta}^*(\cdot) = \arg \min_{\boldsymbol{\theta} \in \Theta} \mathbb{E}[l(Y, G(\boldsymbol{\theta}(\mathbf{X}), \mathbf{T}))]$, where $l(\cdot, \cdot)$ is the loss function (squared error).
- The parameters we are interested in estimating and inferring:
 - Average treatment effect (ATE):** $\mu(\mathbf{t}) = \mathbb{E}[H(\mathbf{X}, \boldsymbol{\theta}^*(\mathbf{X}); \mathbf{t})] = \mathbb{E}[G(\boldsymbol{\theta}^*(\mathbf{X}), \mathbf{t}) - G(\boldsymbol{\theta}^*(\mathbf{X}), \mathbf{t}_o)]$, for all $\mathbf{t} \in \{0,1\}^m$, where $\mathbf{t}_o = (0, 0, \dots, 0)'$.
 - Best-arm identification:** $\mathbf{t}^* = \arg \max_{\mathbf{t} \in \{0,1\}^m} \mu(\mathbf{t})$.
- Two-stage procedure:** (a) training; (b) estimation & inference.

Structured Deep Neural Nets



- Empirical estimator of $\theta^*(.)$:

$$\hat{\theta}(.) = \arg \min_{\theta \in \mathcal{F}_{DNN}} \frac{1}{n} \sum_{i=1}^n l(y_i, G(\theta(x_i), t_i)),$$

which is obtained by SGD or Adam.

Link Function and Convergence

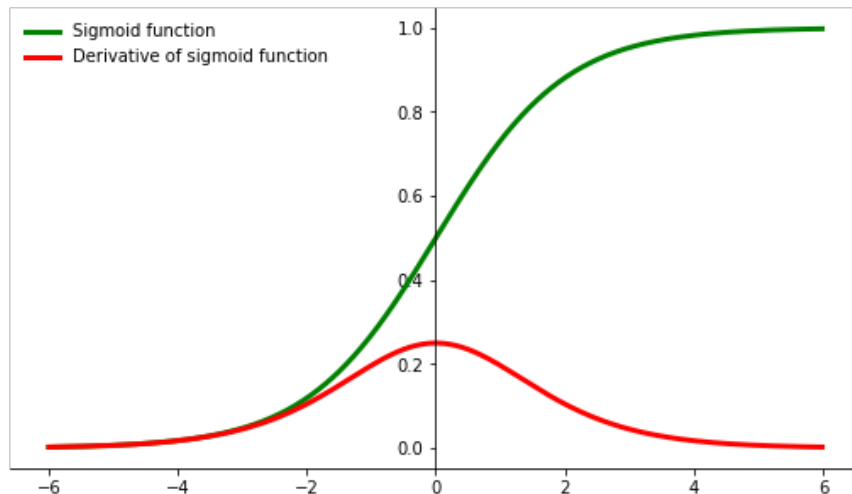
- We adopt the following link function $G(\cdot, \cdot)$ to approximate the true DGP:

- Generalized Sigmoid Function:

$$G(\boldsymbol{\theta}^*(\mathbf{x}), \mathbf{t}) = \frac{\theta_{m+1}^*(\mathbf{x})}{1 + \exp(-(\theta_0^*(\mathbf{x}) + \theta_1^*(\mathbf{x})t_1 + \dots + \theta_m^*(\mathbf{x})t_m))}$$

- $\boldsymbol{\theta}(\mathbf{x})' \mathbf{t}$: The HTE of treatment combination \mathbf{t} with respect to different \mathbf{x} .
- The generalized sigmoid function captures both **diminishing marginal return** and/or **increasing marginal return**, and any possible **ranges** of potential outcomes (by $\theta_{m+1}^*(\cdot)$).

Theorem. Under some **regularity** and **network size** assumptions on \mathcal{F}_{DNN} and the **treatment assignment mechanism** (with $m+2$ **observable combinations**) of the A/B tests, $\hat{\boldsymbol{\theta}}$ converges to $\boldsymbol{\theta}^*$ sufficiently fast $o(n^{-1/4})$ for inference (with subsequent debias).



$$\underbrace{\|\hat{\boldsymbol{\theta}}_k - \boldsymbol{\theta}_k^*\|_{L_2(\mathbf{X})}^2}_{L_2\text{- Norm}} \leq C \left\{ n^{-\frac{p}{p+d_{\mathbf{X}}}} \log^8 n + \frac{\log \log n}{n} \right\}$$

$$\underbrace{\mathbb{E}_n [(\hat{\boldsymbol{\theta}}_k - \boldsymbol{\theta}_k^*)^2]}_{\text{Sample Average}} \leq C \left\{ n^{-\frac{p}{p+d_{\mathbf{X}}}} \log^8 n + \frac{\log \log n}{n} \right\}$$

- p : Smoothness of the DNN class.

Debias with Neyman Orthogonal Score

- The plug-in (PI) estimator for ATE:

$$\hat{\mu}_{PI}(\mathbf{t}) = \frac{1}{n} \sum_{i=1}^n H(\mathbf{x}_i, \hat{\boldsymbol{\theta}}(\mathbf{x}_i); \mathbf{t}) = \frac{1}{n} \sum_{i=1}^n [G(\hat{\boldsymbol{\theta}}(\mathbf{x}_i), \mathbf{t}) - G(\hat{\boldsymbol{\theta}}(\mathbf{x}_i), \mathbf{t}_o)]$$

- A critical issue with the PI estimator:** Insufficient convergence speed to the true ATE (we need **root-N consistency**).
 - Additional **biases** and **inconsistencies** from perturbations of $\hat{\boldsymbol{\theta}}(\cdot)$ because of **regularization** and/or the **variations in \mathbf{X}** .
- Solution: Neyman Orthogonal Score.**
 - Moment conditions:** $\mathbb{E}[\psi(\mathbf{W}, \mu, \boldsymbol{\theta}^*)] = 0$ (ψ is the score function, $\mathbf{W} = (Y, (\mathbf{X}, \mathbf{T})')$ is the data, μ is the ATE, and $\boldsymbol{\theta}^*$ is the true parameter).
 - Neyman Orthogonality:** $\partial_{\boldsymbol{\theta}} \mathbb{E}[\psi(\mathbf{W}, \mu, \boldsymbol{\theta})] |_{\boldsymbol{\theta}=\boldsymbol{\theta}^*} = 0$.
 - Under Neyman orthogonality, even though $\hat{\boldsymbol{\theta}}$ **slightly perturbs** from the true value $\boldsymbol{\theta}^*$, it does not affect the moment conditions.
 - The bias of $\hat{\boldsymbol{\theta}}$ will not affect the moment conditions, so it will not significantly change the subsequent estimator $\hat{\mu}$.

Theorem. Under nonrestrictive regularity assumptions, $\psi(\mathbf{w}, \boldsymbol{\theta}, \boldsymbol{\Lambda}; \mathbf{t}) - \mu(\mathbf{t})$ is a Neyman Orthogonal score, where $\psi(\mathbf{w}, \boldsymbol{\theta}, \boldsymbol{\Lambda}; \mathbf{t}) = H(\mathbf{x}, \boldsymbol{\theta}(\mathbf{x}); \mathbf{t}) - \partial_{\boldsymbol{\theta}} H(\mathbf{x}, \boldsymbol{\theta}(\mathbf{x}); \mathbf{t}) \boldsymbol{\Lambda}(\mathbf{x})^{-1} \partial_{\boldsymbol{\theta}} l(y, G(\boldsymbol{\theta}(\mathbf{x}), \mathbf{t}))$, with $\boldsymbol{\Lambda}(\mathbf{x}) = \mathbb{E}[\partial_{\boldsymbol{\theta}}^2 l(y, G(\boldsymbol{\theta}(\mathbf{x}), \mathbf{t})) | \mathbf{X} = \mathbf{x}]$.



- \mathbf{t} : In the data.
- \mathbf{t} : Want to estimate.

- Remark: The influence function is derived based on the pathwise derivative approach in semi-parametric statistics (Newy 1994, Chernozhukov et al. 2018, Farrell et al. 2020).

Cross-Fitting and Asymptotic Normality

- To avoid over-fitting, we apply cross-fitting:
 - The training set is split into S non-overlapping subsets $S_1, S_2 \dots S_S$. $\hat{\theta}_s$ is trained on S_s^c , the complement of S_s .

$$\psi(\mathbf{w}, \boldsymbol{\theta}, \boldsymbol{\Lambda}; \mathbf{t}) = H(\mathbf{x}, \boldsymbol{\theta}(\mathbf{x}); \mathbf{t}) - \partial_{\boldsymbol{\theta}} H(\mathbf{x}, \boldsymbol{\theta}(\mathbf{x}); \mathbf{t}) \boldsymbol{\Lambda}(\mathbf{x})^{-1} \partial_{\boldsymbol{\theta}} l(y, G(\boldsymbol{\theta}(\mathbf{x}), \mathbf{t}))$$

$$\hat{\mu}(\mathbf{t}) = \frac{1}{S} \sum_{i=1}^S \hat{\mu}_s(\mathbf{t}), \quad \hat{\mu}_s(\mathbf{t}) = \frac{1}{|S_s|} \sum_{j \in S_s} \psi(\mathbf{w}_j, \hat{\boldsymbol{\theta}}_s(\mathbf{x}_j), \hat{\boldsymbol{\Lambda}}_s(\mathbf{x}_j); \mathbf{t})$$

$$\hat{\Psi}(\mathbf{t}) = \frac{1}{S} \sum_{i=1}^S \hat{\Psi}_s(\mathbf{t}), \quad \hat{\Psi}_s(\mathbf{t}) = \frac{1}{|S_s|} \sum_{j \in S_s} (\psi(\mathbf{w}_j, \hat{\boldsymbol{\theta}}_s(\mathbf{x}_j), \hat{\boldsymbol{\Lambda}}_s(\mathbf{x}_j); \mathbf{t}) - \hat{\mu}(\mathbf{t}))^2$$

Theorem. Under nonrestrictive regularity assumptions,

$$\sqrt{n/\hat{\Psi}(\mathbf{t})}(\hat{\mu}(\mathbf{t}) - \mu(\mathbf{t})) \rightarrow_d \mathcal{N}(0,1)$$

- ATE Estimator:** $\hat{\mu}(\mathbf{t})$.
- $(1 - \alpha)$ -Confidence Interval:** $[\hat{\mu}(\mathbf{t}) - z_{1-\frac{\alpha}{2}} \sqrt{\frac{\hat{\Psi}(\mathbf{t})}{n}}, \hat{\mu}(\mathbf{t}) + z_{1-\frac{\alpha}{2}} \sqrt{\frac{\hat{\Psi}(\mathbf{t})}{n}}]$.
- Partial observability:** \mathbf{t} can be an **unobservable** treatment combination.

We call the entire framework as **Debiased Deep Learning (DeDL)**.

Best-Arm Identification

- The true best-arm: $\mathbf{t}^* = \arg \max_{\mathbf{t} \in \{0,1\}^m} \mu(\mathbf{t})$; the estimated best-arm: $\hat{\mathbf{t}}^* = \arg \max_{\mathbf{t} \in \{0,1\}^m} \hat{\mu}(\mathbf{t})$.
- The advantage of $\hat{\mathbf{t}}^*$ over \mathbf{t} : $\tau(\mathbf{t}) := \mu(\hat{\mathbf{t}}^*) - \mu(\mathbf{t})$; the estimator for $\tau(\mathbf{t})$: $\hat{\tau}(\mathbf{t}) = \hat{\mu}(\hat{\mathbf{t}}^*) - \hat{\mu}(\mathbf{t})$.
- The influence function for $\tau(\mathbf{t})$: $\psi(\mathbf{w}, \boldsymbol{\theta}, \Lambda; \hat{\mathbf{t}}^*) - \psi(\mathbf{w}, \boldsymbol{\theta}, \Lambda; \mathbf{t})$, via which the SE of $\hat{\tau}(\mathbf{t})$ can be derived.

Theorem. Under nonrestrictive regularity assumptions, $\hat{\tau}(\mathbf{t})$ is a consistent estimator of $\tau(\mathbf{t})$, and $\sqrt{n} (\hat{\tau}(\mathbf{t}) - \tau(\mathbf{t}))$ converges to a normal distribution.

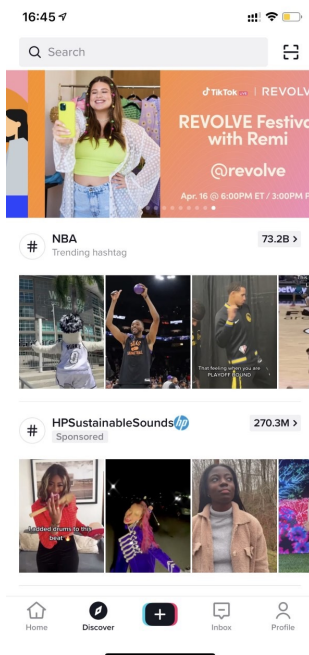
- To verify $\hat{\mathbf{t}}^* = \mathbf{t}^*$, it suffices to do **one-sided tests for the Hypotheses $\tau(\mathbf{t}) > 0$** , where $\mathbf{t} \in \{0,1\}^m$.
- The DeDL framework can be applied to estimating and inferring a wide range of quantities of interest, with the **influence function properly (re-)derived**. Examples:
 - ATE of a personalized policy to adopt **(estimated) optimal treatment combination $\hat{\mathbf{t}}^*$** for each user.
 - Policy evaluation for **any personalized policy π** that maps a user feature \mathbf{x} to a distribution on the treatment space $\{0,1\}^m$.

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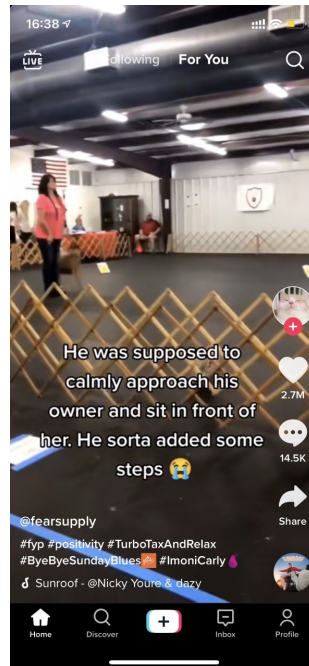
Field Setting



Live Page



Discover Page

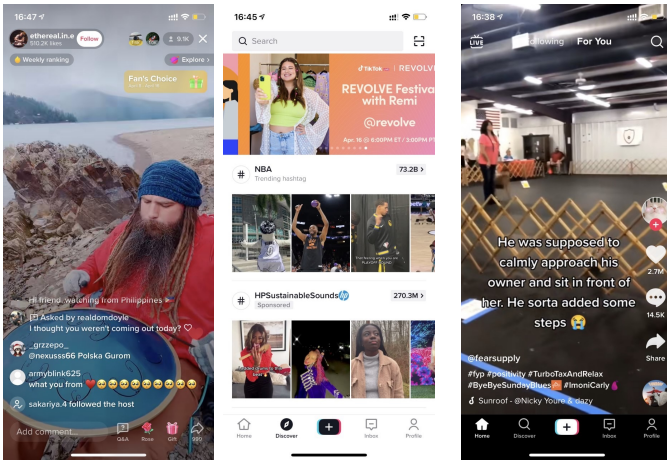


For You Page

- A Chinese online short-video sharing platform (referred to as **Platform O** hereafter).
- **350 million+** DAU, **half-billion+** MAU, **20 million+** USD advertising revenue per day.
- Platform O launches **hundreds of A/B tests** everyday to fast iterate their business operations.
- We consider $m = 3$ major A/B tests on the **algorithmic upgrades** of the 3 pages on the left.

Objective: (a) Estimate and infer ATE; (b) Best-arm identification.

A/B Tests, Data, and Ground-Truth



Live Page Discover Page For You Page

- Duration: Jan 10, 2021-Feb. 01, 2021.
- Sample size: 2,066,606 (roughly 258,325 under each $t \in \{0,1\}^3$)
- Y = Total video-watching time of a user per day.
- X = User demographics (e.g., gender) and pre-treatment behaviors (e.g., the number of active days 1 week before the experiment).
- **Randomization checks** are passed, so users under different treatment combinations are **comparable**.

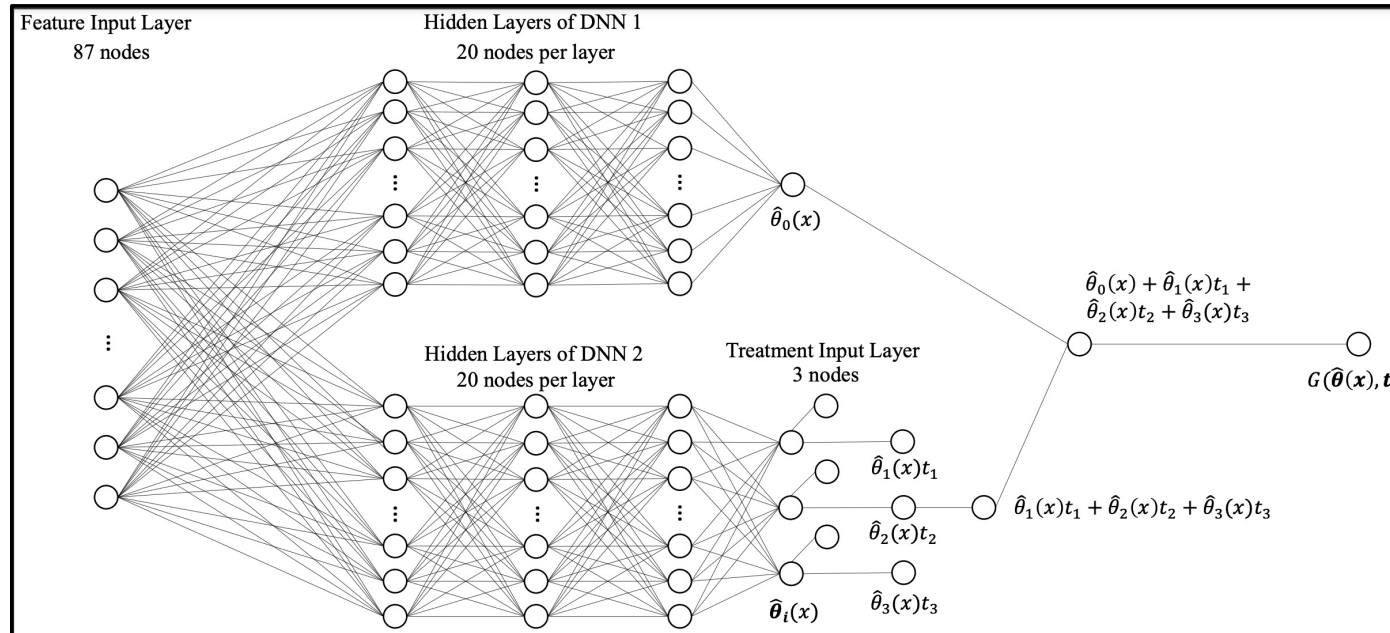
Treatment Combination (t)	Ground-Truth ATE (Scaled)	Observable?	Number of Users
(0,0,0)	0.000%	Observable	258,249
(0,0,1)	1.091%**	Observable	258,340
(0,1,0)	-0.267%	Observable	258,367
(1,0,0)	0.758%*	Observable	258,321
(1,1,1)	2.121%****	Observable	258,375
(1,1,0)	0.689%	Unobservable	258,480
(1,0,1)	2.299%****	Unobservable	258,305
(0,1,1)	1.387%***	Unobservable	258,172

Note:

- Observable means observable for the **estimators**.
- The relative ATEs are reported to protect sensitive data.
- True best-arm: $t^* = (1,0,1)$
- * $p < 0.05$; ** $p < 0.01$; *** $p < 0.001$; **** $p < 0.0001$.

Implementation of the DeDL Framework

- DGP: $\mathbb{E}[Y|X = \mathbf{x}, T = \mathbf{t}] = G(\boldsymbol{\theta}^*(\mathbf{x}), \mathbf{t}) = \frac{\theta_4^*(\mathbf{x})}{1 + \exp(-(\theta_0^*(\mathbf{x}) + \theta_1^*(\mathbf{x})t_1 + \theta_2^*(\mathbf{x})t_2 + \theta_3^*(\mathbf{x})t_3))}$



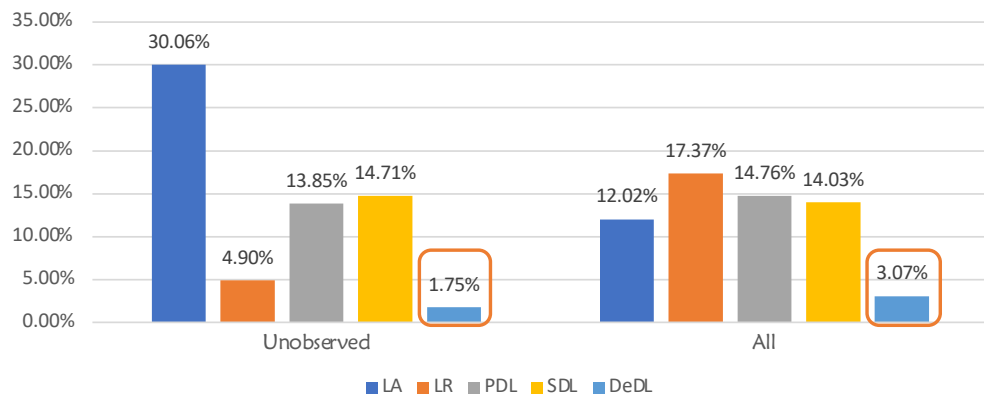
- The DNNs are trained with data from the **observable treatment combinations**.
- One DNN for $\hat{\theta}_0$ (dropout rate=0.1) and the other for $(\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3)$ (dropout rate=0.2). Each has 3 hidden layers; each layer has 20 nodes. All use ReLU as the activation function.
- The third DNN for $\hat{\theta}_4$ is trained as a linear layer.

Benchmarks

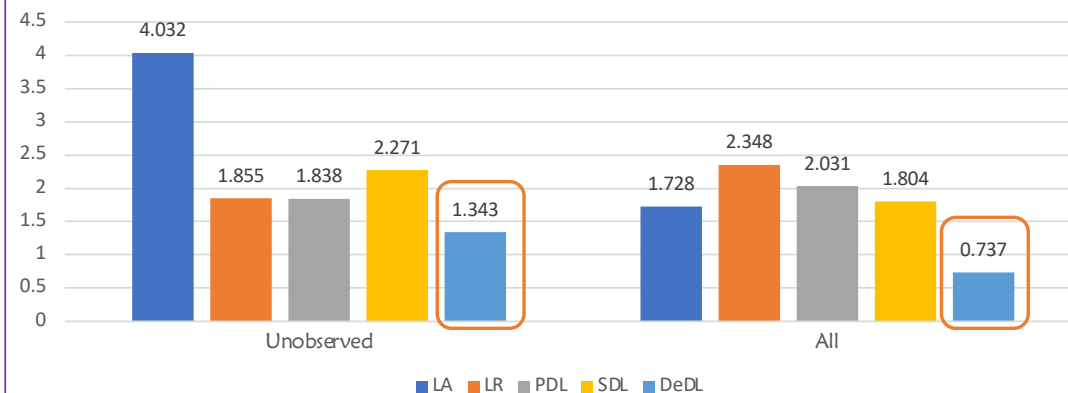
- **Linear Addition (LA):** Assume that the ATE of different individual treatments are **linearly and independently additive**.
 - Effect of “Get Rewards + Send Gift” = Effect of “Get Rewards” + Effect of “Send Gift”
- **Linear Regression (LR):** Regress Y on $(T', X)'$ and predict the outcomes of unobservable treatment combinations by **linear extrapolation**.
 - Still a linear approach, but better leverages the user features.
- **Pure Deep Learning (PDL):** Apply a **generic DNN** with $(T', X)'$ as the inputs to predict the outcomes of unobservable treatment combinations.
 - Fully leverages the predictive power of DNN but without valid inference.
- **Structured Deep Learning (SDL):** Apply **the same DNN as DeDL without debias** to predict the outcomes of unobservable treatment combinations.
 - Comparing DeDL with SDL highlights **the value of bias correction through DML**.

ATE Estimation and Inference

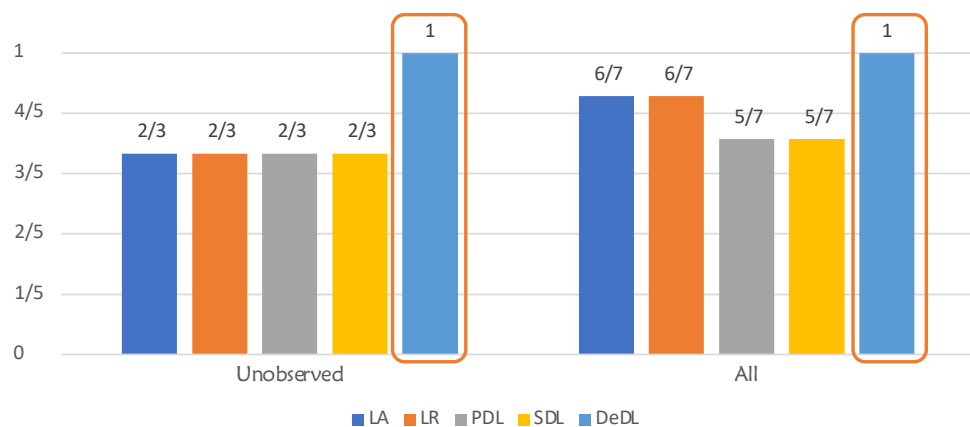
MAPE



MAE

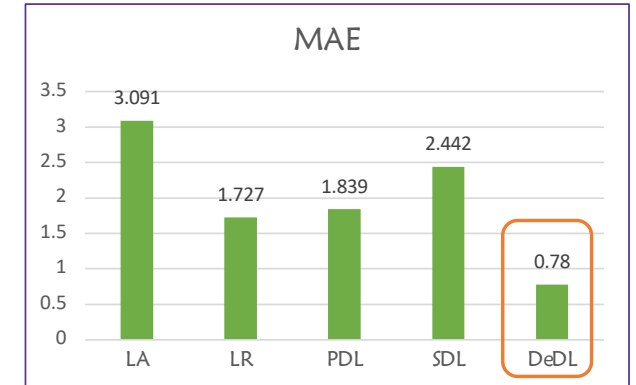
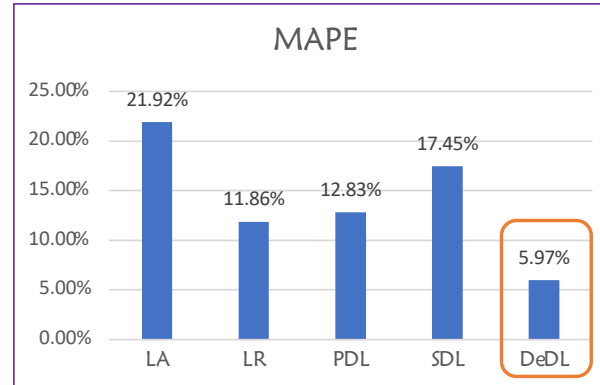
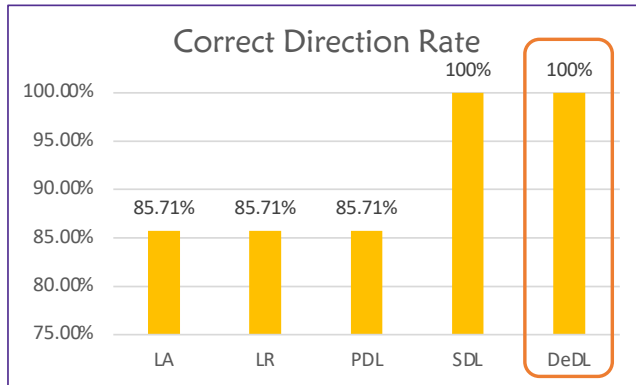


Correct Direction Rate



- The performance metrics are evaluated **against the ground truth ATE** with respect to 3 (resp. 7) **unobservable** (resp. **all**) treatment combinations.
- **Correct Direction** = Correctly identifying the **statistical significance** and **sign** of ATE.
- Key insights:
 - The empirical results **validate DeDL in a field setting!**
 - Naive application of DNNs does **NOT** outperform linear benchmarks.
 - Bias-correction via Neyman orthogonality **substantially improves the performance of DNNs for every treatment combination.**

Best-Arm Identification

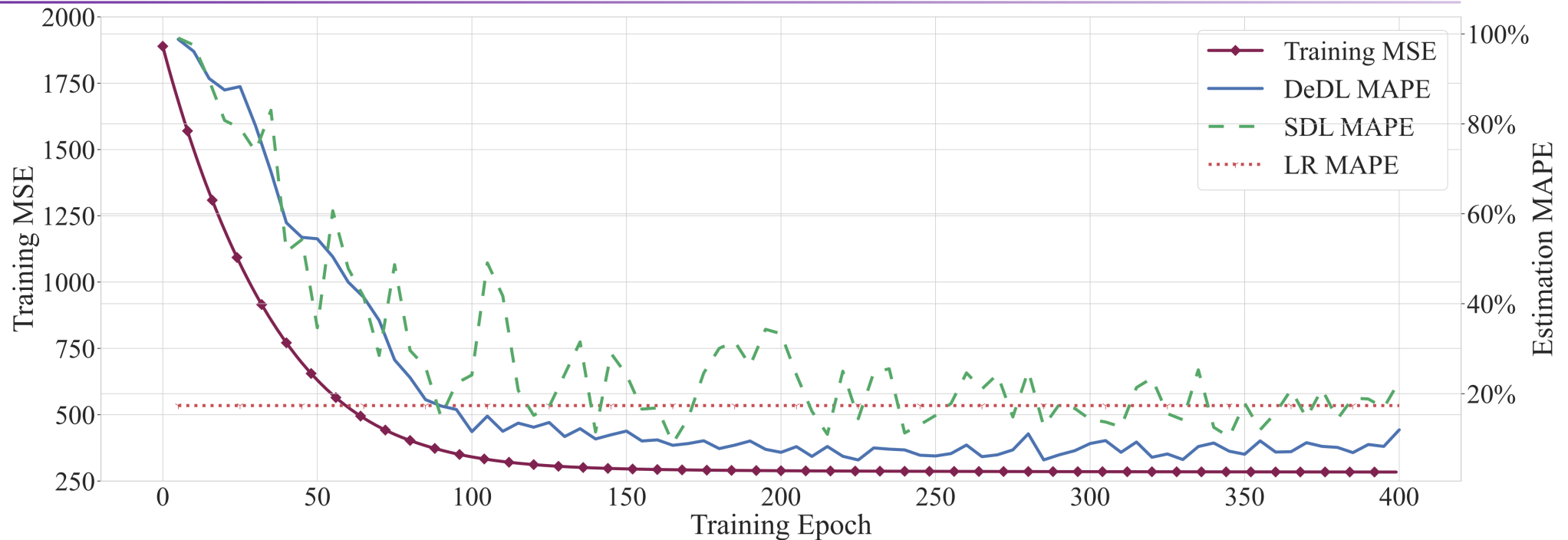


Note:

- We report the CDR, MAPE and MAE of estimating $\tau(\mathbf{t})$ against the ground-truth for LA, LR, PDL, SDL, and DeDL.

- DeDL and SDL can reliably identify the optimal treatment combination, $\hat{\mathbf{t}}^* = \mathbf{t}^* = (1,0,1)$.
- DeDL outperforms the benchmarks for better inferring the advantage of $\hat{\mathbf{t}}^*$ over other treatment combinations.
 - $\tau(\mathbf{t})$'s are more accurately predicted by DeDL.

From Training to Inference



- If the DNN is **not designed and/or not well-trained**, the ATE estimation via DeDL will have a **terrible performance (MAPE > 60%)**.
- If the DNN performs well, DeDL will **consistently beat linear and DL benchmarks without debiasing**.
- The **DNN training error** serves as an important indicator for the **quality of second-stage estimation leveraging debiasing**.

Insights from Synthetic Data

Good News

- The advantage of DeDL **expands** when the number of A/B tests m is larger.
- If the **link function $G(.,.)$ is correctly specified**, DeDL **performs well** even when additional biases are introduced in the **training procedure**.

Bad News

- If the **link function $G(.,.)$ is seriously misspecified**, DeDL may perform poorly.
 - **Vulnerability under model misspecification.**
 - **Model misspecification** can be detected by **DNN training error**.
 - **Recipe:** (i) abandon the debias term; (ii) auto-debias (Chernozhukov et al. 2022).

Takeaways

- **DeDL framework:** A new **DL+DML framework** to estimate and infer the causal effects of multiple A/B tests on large-scale platforms with **unobservable outcomes**.
 - Theoretical valid for inference via **Neyman orthogonality**.
- **Implementation:** **Real large-scale A/B tests (N > 2,000,000)** on Platform O.
 - **Better performance** than the **linear and DL benchmarks** in ATE estimation and best-arm identification.
- **Practice:** Inspirations for future researchers and practitioners to **apply DL+DML** in other important settings for **program evaluation** with **experimental** or **observational data**.



Code: [https://github.com/zikunye2/deep learning based causal inference for combinatorial experiments](https://github.com/zikunye2/deep_learning_based_causal_inference_for_combinatorial_experiments)