Supplementary Materials

A PROOFS

Theorem 4.1

Proof. We'll use the Law of Total Expectation, conditioning on the set of individuals $\mathcal{U}$ selected in the first stage and reasoning about the randomness from the treatment assignments $\mathbf{z}$. We have,

$$\begin{aligned}
\mathop{\mathbb{E}}_{\mathbf{z}}\left[\widehat{\mathrm{TTE}}_{\mathrm{PI}} \,\middle|\, \mathcal{U}\right] &= \tfrac{q}{np}\sum_{t=0}^{\beta} h_{t,q} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^{\beta}} c_{i,\mathcal{S}} \cdot \mathop{\mathbb{E}}_{\mathbf{z}}\Big[\prod_{j\in\mathcal{S}} z_j^t \,\Big|\, \mathcal{U}\Big] \\
&= \tfrac{q}{np}\sum_{t=0}^{\beta} h_{t,q} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^{\beta}} c_{i,\mathcal{S}} \cdot \mathbb{I}(\mathcal{S}\subseteq\mathcal{U}) \cdot \Big[\tfrac{tpn/\beta}{|\mathcal{U}|}\Big]_{|\mathcal{S}|} \\
&= \tfrac{q}{np}\sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^{\beta}} c_{i,\mathcal{S}} \cdot \mathbb{I}(\mathcal{S}\subseteq\mathcal{U}) \sum_{t=0}^{\beta} h_{t,q} \Big[\tfrac{tpn/\beta}{|\mathcal{U}|}\Big]_{|\mathcal{S}|} \\
&= \tfrac{q}{np}\sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^{\beta}} c_{i,\mathcal{S}} \cdot \mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}\big)\Big(1^{|\mathcal{S}|} - 0^{|\mathcal{S}|}\Big) \\
&= \tfrac{q}{np}\sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^{\beta}\setminus\varnothing} c_{i,\mathcal{S}} \cdot \mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}\big) \qquad \text{(A.1)}
\end{aligned}$$

Here, the fourth line follows from the properties of Lagrange interpolation. Note that $h_{t,q} = \ell_{t,\mathbf{x}}(1) - \ell_{t,\mathbf{x}}(0)$, where $\ell_{t,\mathbf{x}}$ is the t'th Lagrange basis polynomial with evaluation points $\mathbf{x} = \big(\frac{tq}{\beta}\big)_{t\in 0,\dots,\beta} = \big(\frac{tpn/\beta}{|\mathcal{U}|}\big)_{t\in 0,\dots,\beta}$. Thus, for any polynomial $f(x)$ with degree at most β,

$$\sum_{t=0}^{\beta} h_{t,q} \cdot f\big(\tfrac{tq}{\beta}\big) = f(1) - f(0).$$

In this case, we let $f(x) = \Big[\frac{x|\mathcal{U}|}{|\mathcal{U}|}\Big]_{|\mathcal{S}|}$, to find that

$$\sum_{t=0}^{\beta} h_{t,q}\Big[\tfrac{tpn/\beta}{|\mathcal{U}|}\Big]_{|\mathcal{S}|} = [1]_{|\mathcal{S}|} - [0]_{|\mathcal{S}|} = 1^{|\mathcal{S}|} - 0^{|\mathcal{S}|}.$$

Now, taking the expectation over the randomness in $\mathcal{U}$, we obtain

$$\begin{aligned}
\mathbb{E}\left[\widehat{\mathrm{TTE}}_{\mathrm{PI}}\right] &= \mathop{\mathbb{E}}_{\mathcal{U}}\Big[\mathop{\mathbb{E}}_{\mathbf{z}}\left[\widehat{\mathrm{TTE}}_{\mathrm{PI}} \,\middle|\, \mathcal{U}\right]\Big] \\
&= \tfrac{1}{n}\sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^{\beta}\setminus\varnothing} c_{i,\mathcal{S}} \cdot \tfrac{q}{p} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}).
\end{aligned}$$

The bias expression in the theorem statement follows from the expression for TTE given in (2.2). ∎

Theorem 4.4

We will use the following algebraic lemma.

Lemma A.1. *For all* $0 < k \leq n_{\mathcal{U}} \leq 1$,

$$|h_{t,q}| = \prod_{\substack{s=0 \\ s\neq t}}^{\beta} \tfrac{\beta/q-s}{t-s} - \prod_{\substack{s=0 \\ s\neq t}}^{\beta} \tfrac{-s}{t-s} \;\leq\; \left(\tfrac{\beta}{q}\right)^{\beta}.$$

Proof. When $\beta = 1$, $|h_{0,q}| = |h_{1,q}| = \frac{1}{q}$, so the inequality holds (with equality). Thus, we can restrict our attention to $\beta \geq 2$, for which we consider in two cases. First, if $t \geq 1$, we have

$$\left|h_{t,q}\right| = \left|\prod_{\substack{s=0 \\ s\neq t}}^{\beta} \tfrac{\beta/q-s}{t-s}\right| \leq \left(\tfrac{\beta}{q}\right)^{\beta}.$$

The equality uses the definition of $h_{t,q}$, and the inequality upper bounds the numerator of each factor with β/q and lower bounds the denominator of each factor by 1. When $t = 0$, we apply the triangle inequality to conclude that

$$\left|h_{0,q}\right| = \left|\prod_{s=1}^{\beta} \tfrac{\beta/q-s}{-s} - 1\right| \leq \prod_{s=1}^{\beta} \tfrac{\beta}{sq} + 1 = \tfrac{1}{\beta!}\left(\frac{\beta}{q}\right)^{\beta} + 1.$$

Since $\beta \geq 2$ and $q \leq 1$, we must have $1 \leq \frac{1}{2}\left(\frac{\beta}{q}\right)^{\beta}$. Thus we can upper-bound this last expression by

$$\tfrac{1}{\beta!}\left(\frac{\beta}{q}\right)^{\beta} + \tfrac{1}{2}\left(\tfrac{\beta}{q}\right)^{\beta} = \left(\tfrac{1}{\beta!} + \tfrac{1}{2}\right) \cdot \left(\frac{\beta}{q}\right)^{\beta} \leq \left(\frac{\beta}{q}\right)^{\beta}.$$

$\square$

We also prove a slightly stronger version of Theorem 3 from Cortez et al. (2022) with the constants specified. It first relies on a slightly modified version of Lemma 8 from Cortez et al. (2022).

Lemma A.2. *For any* $x \in (0, 1]$ *and any constants* $a, b \in \mathbb{N}$ *such that* $xn \geq \sqrt{2}ab + b - 1$,

$$\left|\frac{\left[\frac{xn-a}{n-a}\right]_b}{\left[\frac{xn}{n}\right]_b} - 1\right| \leq \tfrac{2ab}{xn-b+1},$$

Proof. First, let us note that when $a = 0$ or $b = 0$, both sides of this inequality simplify to 0, so it holds with equality. Thus, we assume throughout the rest of the proof that $a, b > 0$. Note that our assumption $xn \geq \sqrt{2}ab + b - 1$ with $x \leq 1$ implies that $n \geq a + b - 1$.

Now, given any any $i \in \{0, \dots, b-1\}$,

$$\frac{xn-a-i}{n-a-i} \leq \frac{xn-i}{n-i} \quad\Rightarrow\quad \frac{\left[\frac{xn-a}{n-a}\right]_b}{\left[\frac{xn}{n}\right]_b} \leq 1.$$

As a result, expanding the bracket notation, we have,

$$\begin{aligned}
\left|\frac{\left[\frac{xn-a}{n-a}\right]_b}{\left[\frac{xn}{n}\right]_b} - 1\right| &= 1 - \prod_{i=0}^{b-1}\Big(\frac{xn-a-i}{xn-i}\Big)\Big(\frac{n-i}{n-a-i}\Big) \\
&= 1 - \prod_{i=0}^{b-1}\Big(1 - \frac{a}{xn-i}\Big)\underbrace{\Big(1 + \frac{a}{n-a-i}\Big)}_{\geq 1}
\end{aligned}$$

$$
\begin{aligned}
&\leq 1 - \prod_{i=0}^{b-1} \Big(1 - \frac{a}{xn - b + 1}\Big) && (i \leq b-1) \\
&= -\sum_{j=1}^{b} \binom{b}{j} \Big(-\frac{a}{(xn-b+1)}\Big)^j && \text{(binomial expansion)} \\
&\leq \sum_{j=1}^{b} \binom{b}{j} \Big(\frac{a}{(xn-b+1)}\Big)^j \cdot \mathbb{I}(j \text{ is odd}) \\
&\leq \Big(\frac{ab}{xn-b+1}\Big) \sum_{j=0}^{\lfloor (b-1)/2 \rfloor} \Big(\frac{ab}{xn-b+1}\Big)^{2j} \\
&\leq \Big(\frac{ab}{xn-b+1}\Big) \sum_{j=0}^{\lfloor (b-1)/2 \rfloor} \Big(\frac{1}{\sqrt{2}}\Big)^{2j} && (xn \geq \sqrt{2}ab + b - 1) \\
&\leq \frac{2ab}{xn-b+1}. && \text{(geometric series with factor } \tfrac{1}{2})
\end{aligned}
$$

□

We use this to lemma to give an upper bound on the covariance of two sets being treated under a CRD rollout design with $\frac{ptn}{\beta}$ individuals treated in round t for each $t \in \{0, \dots, \beta\}$.

Lemma A.3. *If $\frac{pt'n}{\beta} \geq 2\beta^2 + \beta - 1$, then for $t \leq t'$ and $\mathcal{S} \cap \mathcal{S}' = \emptyset$ with $|\mathcal{S}|, |\mathcal{S}'| \geq 1$, it follows that*

$$\Big|\mathrm{Cov}\Big[\prod_{j \in \mathcal{S}} z_j^t, \prod_{j' \in \mathcal{S}'} z_{j'}^{t'}\Big]\Big| \leq \frac{4p\beta^3}{n}.$$

Proof. First, let us note that if $t = 0$, then the first argument of this covariance is not random, so the covariance simplifies to 0, trivially satisfying the bound. Thus, we may assume that $1 \leq t \leq t'$. We can rewrite the covariance expression:

$$
\begin{aligned}
\Big|\mathrm{Cov}\Big[\prod_{j \in \mathcal{S}} z_j^t, \prod_{j' \in \mathcal{S}'} z_{j'}^{t'}\Big]\Big| &= \Big|\mathbb{E}\Big[\prod_{j \in \mathcal{S}} z_j^t \prod_{j' \in \mathcal{S}'} z_{j'}^{t'}\Big] - \mathbb{E}\Big[\prod_{j \in \mathcal{S}} z_j^t\Big] \mathbb{E}\Big[\prod_{j' \in \mathcal{S}'} z_{j'}^{t'}\Big]\Big| \\
&= \Big[\tfrac{ptn/\beta}{n}\Big]_{|\mathcal{S}|} \Big[\tfrac{pt'n/\beta}{n}\Big]_{|\mathcal{S}'|} \cdot \left| \frac{\Big[\frac{pt'n/\beta - |\mathcal{S}|}{n - |\mathcal{S}|}\Big]_{|\mathcal{S}'|}}{\Big[\frac{pt'n/\beta}{n}\Big]_{|\mathcal{S}'|}} - 1 \right|.
\end{aligned}
$$

We can bound this last absolute value expression using Lemma A.2, letting $x = pt'/\beta$, $a = |\mathcal{S}|$, and $b = |\mathcal{S}'|$. Note that $a, b \leq \beta$, so our assumption that $\frac{pt'n}{\beta} \geq 2\beta^2 + \beta - 1$ ensures that $xn \geq \sqrt{2}ab + b - 1$. We find that

$$\Big|\mathrm{Cov}\Big[\prod_{j \in \mathcal{S}} z_j^t, \prod_{j' \in \mathcal{S}'} z_{j'}^{t'}\Big]\Big| \leq \Big(\tfrac{pt}{\beta}\Big)^{|\mathcal{S}|} \Big(\tfrac{pt'}{\beta}\Big)^{|\mathcal{S}'|} \cdot \frac{2|\mathcal{S}||\mathcal{S}'|}{\frac{pt'n}{\beta} - |\mathcal{S}'| + 1} \leq \frac{2p^2\beta^3}{pn - \beta^2} \leq \frac{4p\beta^3}{n}$$

Here, the final equality uses the fact that $pn \geq pt'n/\beta \geq 2\beta^2$ to conclude that $\frac{p}{pn - \beta^2} \leq \frac{2}{n}$. □

When $\mathcal{S} \cap \mathcal{S}' \neq \emptyset$ for $|\mathcal{S}|, |\mathcal{S}'| \geq 1$, it follows that

$$\Big|\mathrm{Cov}\Big[\prod_{j \in \mathcal{S}} z_j^t, \prod_{j' \in \mathcal{S}'} z_{j'}^{t'}\Big]\Big| \leq p.$$

Plugging this into Lemma 6 of Cortez et al. (2022), (so, in their notation, $\alpha = \big(\frac{\beta}{p}\big)^\beta$, $B_1 = p$, and $B_2 = \frac{4p\beta^3}{n}$), we can upper bound the variance of the staggered rollout estimator under a CRD rollout design by

$$\mathrm{Var}\big(\widehat{\mathrm{TTE}}\big) \leq \frac{\beta^2 Y_{\max}^2 p}{n} \cdot \Big(\tfrac{\beta}{p}\Big)^{2\beta} \cdot \Big(d^2 + 4\beta^3\Big). \tag{A.2}$$

Please Note: There is a small typo in the variance bound given in the statement of this theorem in the paper body. A correct bound, which is proven below is

$$\mathrm{Var}\left(\widehat{\mathrm{TTE}}\right) \le \mathbb{I}(q<1)\cdot \tfrac{q^3\beta^2 Y_{\max}^2}{p^2 n}\left(\tfrac{\beta}{q}\right)^{2\beta}\left(d^2+4\beta^3\right) + \tfrac{q-p}{p(n_c-1)}\widehat{\mathrm{Var}}(\bar{L}_\pi) + \mathbb{I}(q>p)\cdot\left(\tfrac{\beta d}{n_c}+\tfrac{d^2}{n_c}\right)\cdot Y_{\max}\cdot C(\delta(\Pi)).$$

We will correct the statement in the final version of the paper. Importantly, the interpretation of this variance bound remains the same.

Proof of Theorem 4.4.

By the Law of Total Variance, we have

$$\underset{\mathbf{z}}{\mathrm{Var}}\left(\widehat{\mathrm{TTE}}\right) = \underset{\mathcal{U}}{\mathbb{E}}\left[\underset{\mathbf{z}|\mathcal{U}}{\mathrm{Var}}\left(\widehat{\mathrm{TTE}}\right)\right] + \underset{\mathcal{U}}{\mathrm{Var}}\left(\underset{\mathbf{z}}{\mathbb{E}}\left[\widehat{\mathrm{TTE}}\mid\mathcal{U}\right]\right).$$

We separately bound each of these terms.

<u>First Term:</u>

First, let us note that when $q=1$, $h_{0,q}=-1$, $h_{\beta,q}=1$ and $h_{t,q}=0$ for all $0<t<\beta$. In this case, we may simplify the estimator to

$$\widehat{\mathrm{TTE}} = \tfrac{1}{np}\sum_{i=1}^{n} Y_i(\mathbf{z}^\beta) - Y_i(\mathbf{z}^0).$$

Conditioned on $\mathcal{U}$, this quantity is deterministic, since $z_j^\beta = \mathbb{I}(j\in\mathcal{U})$ and $z_j^0=0$. Thus, the variance of the estimator conditioned on $\mathcal{U}$ is 0, making the first term of our variance expression 0. Thus, we may restrict our attention to the case when $q<1$ and multiply the resulting expression by the indicator $\mathbb{I}(q<1)$ in our final bound.

Now, let $\tilde{\mathbf{z}}\sim\mathrm{CRD}(qn,n)$ be a random vector with $z_j^t = \tilde{z}_j^t\cdot\mathbb{I}(j\in\mathcal{U})$. Conditioned on $\mathcal{U}$, we may rewrite our estimator:

$$\begin{aligned}
\widehat{\mathrm{TTE}} &= \tfrac{q}{np}\sum_{t=0}^{\beta} h_{t,q}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta} c_{i,\mathcal{S}}\prod_{j\in\mathcal{S}} z_j^t \\
&= \sum_{t=0}^{\beta} h_{t,q}\cdot\left(\tfrac{1}{n}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta}\tfrac{q}{p}\cdot c_{i,\mathcal{S}}\cdot\mathbb{I}(\mathcal{S}\subseteq\mathcal{U})\prod_{j\in\mathcal{S}}\tilde{z}_j^t\right) \\
&= \sum_{t=0}^{\beta} h_{t,q}\cdot\left(\tfrac{1}{n}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta}\tilde{c}_{i,\mathcal{S}}\prod_{j\in\mathcal{S}}\tilde{z}_j^t\right) \\
&= \sum_{t=0}^{\beta} h_{t,q}\cdot\left(\tfrac{1}{n}\sum_{i=1}^{n}\tilde{Y}_i(\tilde{\mathbf{z}}^t)\right),
\end{aligned}$$

where

$$\tilde{c}_{i,\mathcal{S}} = \tfrac{q}{p}c_{i,\mathcal{S}}\cdot\mathbb{I}(\mathcal{S}\subseteq\mathcal{U}), \qquad \tilde{Y}_i(\tilde{\mathbf{z}}) = \sum_{\mathcal{S}\in\mathcal{S}_i^\beta}\tilde{c}_{i,\mathcal{S}}\prod_{j\in\mathcal{S}}\tilde{z}_j^t.$$

Writing it in this way, we can see that the distribution of $\widehat{\mathrm{TTE}}$ conditioned on $\mathcal{U}$ is equivalent to the distribution of the polynomial interpolation estimator in Cortez et al. (2022) with $\tilde{\mathbf{z}}\sim\mathrm{CRD}(qn,n)$ for a modified potential outcomes model given by the coefficients $\tilde{c}_{i,\mathcal{S}}$.

Under the assumption that $c_{i,\mathcal{S}}\ge 0$, then $\tilde{Y}_i(\mathbf{z})\le\frac{q}{p}Y_i(\mathbf{z})$.

As a result, the variance of $\widehat{\mathrm{TTE}}$ conditioned on $\mathcal{U}$ can be upper-bounded from (A.2). As this expression does not depend on $\mathcal{U}$,

$$\underset{\mathcal{U}}{\mathbb{E}}\left[\underset{\mathbf{z}|\mathcal{U}}{\mathrm{Var}}\left(\widehat{\mathrm{TTE}}\right)\right] \le \tfrac{q^3\beta^2Y_{\max}^2}{p^2n}\cdot\left(\tfrac{\beta}{q}\right)^{2\beta}\cdot\left(d^2+4\beta^3\right).$$

Second Term:

First, let us note that when $q = p$, every individual is deterministically included in $\mathcal{U}$ during Stage 1 of the experiment. In this case, the second term, which concerns a variance over $\mathcal{U}$, is 0. Thus, we may restrict our attention to the case when $q > p$ and multiply the resulting expression by the indicator $\mathbb{I}(q > p)$ in our final bound.

We first split $\mathbb{E}_{\mathbf{z}}\left[\widehat{\mathrm{TTE}}_{\mathrm{PI}} \,\middle|\, \mathcal{U}\right]$ from (A.1) into the terms associated to sets $\mathcal{S}$ that are fully contained inside a cluster as opposed to sets $\mathcal{S}$ that contain members of more than one cluster.

$$\mathbb{E}_{\mathbf{z}}\left[\widehat{\mathrm{TTE}}_{\mathrm{PI}} \,\middle|\, \mathcal{U}\right] = \tfrac{q}{np}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}, |\Pi(\mathcal{S})|=1\big) + \tfrac{q}{np}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}, |\Pi(\mathcal{S})|\geq 2\big). \tag{A.3}$$

We may rewrite the first term of (A.3):

$$\tfrac{q}{np}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}, |\Pi(\mathcal{S})|=1\big) \quad=\quad \tfrac{q}{np}\sum_{i=1}^{n}\sum_{\pi\in\Pi} x_\pi \sum_{\substack{\mathcal{S}\in\mathcal{S}_i^\beta \\ \mathcal{S}\neq\varnothing}} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(S\subseteq\pi\big) \quad=\quad \tfrac{q}{pn_c}\sum_{\pi\in\Pi} x_\pi \bar{L}_\pi,$$

where $x_\pi = \mathbb{I}\big(\pi\subseteq\mathcal{U}\big)$ and $\bar{L}_\pi$ is defined as in the main text, with

$$\bar{L}_\pi = \tfrac{n_c}{n}\sum_{i=1}^{n}\sum_{\mathcal{S}\subseteq[n]} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(\mathcal{S}\subseteq\pi\big),$$

which represents the effects associated with sets fully contained inside cluster π. In Stage 1, we select clusters according to a CRD design. In particular, $\mathbf{x}\sim\mathrm{CRD}(pn_c/q, n_c)$. Applying Lemma 4.5, we find that the variance of the first term of (A.3) is equal to

$$\tfrac{q-p}{p(n_c-1)}\cdot\widehat{\mathrm{Var}}\big(\bar{L}_\pi\big).$$

To upper bound the terms of the variance associated to the second term of $\mathbb{E}_{\mathbf{z}}\left[\widehat{\mathrm{TTE}}_{\mathrm{PI}} \,\middle|\, \mathcal{U}\right]$ associated to all the sets $\mathcal{S}$ for which $|\Pi(\mathcal{S})|\geq 2$, we use the bound that for any $\mathcal{S}$ such that $|\Pi(\mathcal{S})|\geq 2$,

$$\mathrm{Cov}\Big(\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}\big), \mathbb{I}\big(\mathcal{S}'\subseteq\mathcal{U}\big)\Big) \leq \Pr(\mathcal{S}\subseteq\mathcal{U})\cdot\mathbb{I}\Big(\Pi(\mathcal{S})\cap\Pi(\mathcal{S}')\neq\emptyset\Big).$$

In addition, we'll make use of our assumption that each $c_{i\mathcal{S}}\geq 0$. Plugging in these bounds, it follows that

$$\begin{aligned}
&\mathrm{Cov}\left(\tfrac{q}{np}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}, |\Pi(\mathcal{S})|\geq 2\big), \tfrac{q}{pn_c}\sum_{\pi\in\Pi} x_\pi\bar{L}_\pi\right) \\
&= \tfrac{q^2}{nn_cp^2}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(|\Pi(\mathcal{S})|\geq 2\big)\sum_{\pi\in\Pi}\bar{L}_\pi\,\mathrm{Cov}(\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}\big), x_\pi) \\
&\leq \tfrac{q^2}{nn_cp^2}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\mathbb{I}\big(|\Pi(\mathcal{S})|\geq 2\big)\sum_{\pi\in\Pi}\bar{L}_\pi\cdot\Pr(\mathcal{S}\subseteq\mathcal{U})\cdot\mathbb{I}(c\in\Pi(\mathcal{S})) \\
&= \tfrac{q^2}{p^2nn_c}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\Pr(\mathcal{S}\subseteq\mathcal{U})\cdot\mathbb{I}\big(|\Pi(\mathcal{S})|\geq 2\big)\sum_{\pi\in\Pi(\mathcal{S})}\bar{L}_\pi \\
&= \tfrac{q^2}{p^2n^2}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\Pr(\mathcal{S}\subseteq\mathcal{U})\cdot\mathbb{I}\big(|\Pi(\mathcal{S})|\geq 2\big)\sum_{\pi\in\Pi(\mathcal{S})}\sum_{i'\in[n]}\sum_{\mathcal{S}'\in\mathcal{S}_i'^\beta} c_{i',\mathcal{S}'}\cdot\mathbb{I}\big(\mathcal{S}'\subseteq\pi\big) \\
&\leq \tfrac{q^2}{p^2n^2}\sum_{i=1}^{n}\sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}}\cdot\Pr(\mathcal{S}\subseteq\mathcal{U})\cdot\mathbb{I}\big(|\Pi(\mathcal{S})|\geq 2\big)\sum_{\pi\in\Pi(\mathcal{S})}\sum_{i'\in[n]}\mathbb{I}\big(\pi\in\Pi(\mathcal{N}_{i'})\big)\sum_{\mathcal{S}'\in\mathcal{S}_i'^\beta} c_{i',\mathcal{S}'}
\end{aligned}$$

$$
\begin{aligned}
&\le \tfrac{q^2 Y_{\max}}{p^2 n^2} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \sum_{\pi\in\Pi(\mathcal{S})} \sum_{i'\in[n]} \mathbb{I}\big(\pi\in\Pi(\mathcal{N}_{i'})\big) \\
&\le \tfrac{q^2 Y_{\max}}{p^2 n^2} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \sum_{\pi\in\Pi(\mathcal{S})} \tfrac{nd}{n_c} \\
&= \tfrac{q^2 d\beta Y_{\max}}{p^2 n_c} \left(\tfrac{1}{n} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \right).
\end{aligned}
$$

In addition,

$$
\begin{aligned}
&\mathrm{Var}\left(\tfrac{q}{np} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}, |\Pi(\mathcal{S})| \ge 2\big) \right) \\
&= \tfrac{q^2}{n^2p^2} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \sum_{i'=1}^{n} \sum_{\mathcal{S}'\in\mathcal{S}_{i'}^\beta\setminus\varnothing} c_{i',\mathcal{S}'} \cdot \mathbb{I}\big(|\Pi(\mathcal{S}')| \ge 2\big) \cdot \mathrm{Cov}\left(\mathbb{I}\big(\mathcal{S}\subseteq\mathcal{U}\big), \mathbb{I}\big(\mathcal{S}'\subseteq\mathcal{U}\big) \right) \\
&\le \tfrac{q^2}{n^2p^2} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \sum_{i'=1}^{n} \sum_{\mathcal{S}'\in\mathcal{S}_{i'}^\beta\setminus\varnothing} c_{i',\mathcal{S}'} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\Big(\Pi(\mathcal{S})\cap\Pi(\mathcal{S}') \ne \emptyset\Big) \\
&\le \tfrac{q^2}{p^2n^2} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \sum_{i'=1}^{n} \mathbb{I}\Big(\Pi(\mathcal{N}_i)\cap\Pi(\mathcal{N}_i') \ne \emptyset\Big) \sum_{\mathcal{S}'\in\mathcal{S}_{i'}^\beta\setminus\varnothing} c_{i',\mathcal{S}'} \\
&\le \tfrac{q^2 Y_{\max}}{p^2 n} \left(\tfrac{1}{n} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \sum_{i'=1}^{n} \mathbb{I}\Big(\Pi(\mathcal{N}_i)\cap\Pi(\mathcal{N}_i') \ne \emptyset\Big) \right) \\
&\le \tfrac{q^2 d^2 Y_{\max}}{p^2 n_c} \left(\frac{1}{n} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \Pr(\mathcal{S}\subseteq\mathcal{U}) \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \right).
\end{aligned}
$$

Putting it all together, we get that

$$
\begin{aligned}
\mathop{\mathrm{Var}}_{\mathcal{U}}\left[\mathop{\mathbb{E}}_{\mathbf{z}}\left(\widehat{\mathrm{TTE}}_{\mathrm{PI}} \mid \mathcal{U} \right) \right] &\le \tfrac{q-p}{p(n_c-1)} \cdot \widehat{\mathrm{Var}}\big(\bar{L}_\pi\big) + \left(\tfrac{d\beta Y_{\max}}{n_c} + \tfrac{d^2 Y_{\max}}{n_c} \right) \left(\tfrac{q^2}{p^2 n} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \right) \\
&\le \tfrac{q-p}{p(n_c-1)} \cdot \widehat{\mathrm{Var}}\big(\bar{L}_\pi\big) + \left(\tfrac{d\beta}{n_c} + \tfrac{d^2}{n_c} \right) Y_{\max} \left(\tfrac{1}{n} \sum_{i=1}^{n} \sum_{\mathcal{S}\in\mathcal{S}_i^\beta\setminus\varnothing} c_{i,\mathcal{S}} \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \right) \\
&\le \tfrac{q-p}{p(n_c-1)} \cdot \widehat{\mathrm{Var}}\big(\bar{L}_\pi\big) + \left(\tfrac{d\beta}{n_c} + \tfrac{d^2}{n_c} \right) \cdot Y_{\max} C(\delta(\Pi)) \\
&\le \tfrac{q-p}{p(n_c-1)} \cdot \widehat{\mathrm{Var}}\big(\bar{L}_\pi\big) + \tfrac{2d^2}{n_c} \cdot Y_{\max} C(\delta(\Pi)).
\end{aligned}
$$

Here, the second inequality uses the fact that

$$
\Pr(\mathcal{S}\subseteq\mathcal{U}) \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big) \le (p/q)^2 \cdot \mathbb{I}\big(|\Pi(\mathcal{S})| \ge 2\big).
$$

□

Theorem 4.6

Proof. When $\beta = 1$, the estimator simplifies to

$$
\widehat{\mathrm{TTE}} = \tfrac{1}{np} \sum_{i\in[n]} \Big(Y_i(\mathbf{z}^1) - Y_i(\mathbf{0}) \Big) = \tfrac{1}{np} \sum_{j\in[n]} L_j z_j^1 = \tfrac{1}{np} \sum_{\pi} \sum_{j\in\pi} L_j z_j^1.
$$

Conditioning on $\mathcal{U}$, the estimator becomes

$$\tfrac{1}{np}\sum_{j\in\mathcal{U}} L_j z_j^1 = \tfrac{1}{q|\mathcal{U}|}\sum_{j\in\mathcal{U}} L_j z_j^1,$$

where here we use the fact that $|\mathcal{U}| = \frac{np}{q}$. Since $\mathbf{z}_{\mathcal{U}} \sim \mathrm{CRD}(q|\mathcal{U}|, q)$, we may use Lemma 4.5 to obtain an expression for the conditional variance:

$$\operatorname*{Var}_{\mathbf{z}|\mathcal{U}}\big(\widehat{\mathrm{TTE}}_{\mathrm{PI}}\big) = \tfrac{1-q}{q(|\mathcal{U}|-1)}\cdot\bigg[\tfrac{1}{|\mathcal{U}|}\sum_{j\in\mathcal{U}} L_j^2 \;-\; \Big(\tfrac{1}{|\mathcal{U}|}\sum_{j\in\mathcal{U}} L_j\Big)^2\bigg].$$

Taking the expectation of this conditional variance with respect to $\mathcal{U}$, we have

$$\begin{aligned}
\mathop{\mathbb{E}}_{\mathcal{U}}\Big[\operatorname*{Var}_{\mathbf{z}|\mathcal{U}}\big(\widehat{\mathrm{TTE}}_{\mathrm{PI}}\big)\Big] &= \tfrac{1-q}{q(|\mathcal{U}|-1)}\bigg[\tfrac{1}{|\mathcal{U}|}\sum_{j\in[n]} L_j^2\cdot\Pr(j\in\mathcal{U}) \;-\; \tfrac{1}{|\mathcal{U}|^2}\sum_{j\in[n]}\sum_{j'\in[n]} L_jL_{j'}\cdot\Pr(j,j'\in\mathcal{U})\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\tfrac{q}{np}\sum_{j\in[n]} L_j^2\cdot\Pr(j\in\mathcal{U}) \;-\; \tfrac{q^2}{n^2p^2}\sum_{j\in[n]}\sum_{j'\in[n]} L_jL_{j'}\cdot\Pr(j,j'\in\mathcal{U})\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\tfrac{1}{n}\sum_{j\in[n]} L_j^2 - \tfrac{q}{n^2p}\sum_{j\in[n]}\sum_{j'\in\pi(j)} L_jL_{j'} - \tfrac{pn_c-q}{n^2p(n_c-1)}\sum_{j\in[n]}\sum_{j'\notin\pi(j)} L_jL_{j'}\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\tfrac{1}{n}\sum_{j\in[n]} L_j^2 - \tfrac{q}{n^2p}\sum_{\pi\in\Pi}\Big(\sum_{j\in\pi} L_j\Big)^2 - \tfrac{pn_c-q}{n^2p(n_c-1)}\bigg[\Big(\sum_{\pi\in\Pi}\sum_{j\in\pi} L_j\Big)^2 - \sum_{\pi\in\Pi}\Big(\sum_{j\in\pi} L_j\Big)^2\bigg]\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\tfrac{1}{n}\sum_{j\in[n]} L_j^2 - \tfrac{q}{n^2p}\sum_{\pi\in\Pi}\Big(\sum_{j\in\pi} L_j\Big)^2 - \tfrac{pn_c-q}{n^2p(n_c-1)}\Big(\sum_{j\in[n]} L_j\Big)^2 + \tfrac{pn_c-q}{n^2p(n_c-1)}\sum_{\pi\in\Pi}\Big(\sum_{j\in\pi} L_j\Big)^2\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\tfrac{1}{n}\sum_{j\in[n]} L_j^2 + \tfrac{(p-q)n_c}{n^2p(n_c-1)}\sum_{\pi\in\Pi}\Big(\sum_{j\in\pi} L_j\Big)^2 - \tfrac{pn_c-q}{p(n_c-1)}\Big(\tfrac{1}{n}\sum_{j\in[n]} L_j\Big)^2\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\bigg[\tfrac{1}{n}\sum_{j\in[n]} L_j^2 - \Big(\tfrac{1}{n}\sum_{j\in[n]} L_j\Big)^2\bigg] + \tfrac{p-q}{p(n_c-1)}\cdot\tfrac{1}{n_c}\sum_{\pi\in\Pi}\Big(\tfrac{n_c}{n}\sum_{j\in\pi} L_j\Big)^2 - \tfrac{p-q}{p(n_c-1)}\Big(\tfrac{1}{n_c}\sum_{\pi\in\Pi}\tfrac{n_c}{n}\sum_{j\in\pi} L_j\Big)^2\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\operatorname*{\widehat{Var}}_{j\in[n]}\big(L_j\big) + \tfrac{p-q}{p(n_c-1)}\bigg[\tfrac{1}{n_c}\sum_{\pi\in\Pi}\big(\bar{L}_\pi\big)^2 - \Big(\tfrac{1}{n_c}\sum_{\pi\in\Pi}\bar{L}_\pi\Big)^2\bigg]\bigg] \\
&= \tfrac{1-q}{np-q}\bigg[\operatorname*{\widehat{Var}}_{j\in[n]}\big(L_j\big) + \tfrac{p-q}{p(n_c-1)}\cdot\operatorname*{\widehat{Var}}_{\pi\in\Pi}\big(\bar{L}_\pi\big)\bigg].
\end{aligned}$$

The conditional expectation is given by

$$\mathop{\mathbb{E}}_{\mathbf{z}}\big[\widehat{\mathrm{TTE}}\;\big|\;\mathcal{U}\big] = \tfrac{q}{pn_c}\sum_{\pi\in\Pi}\Big(\tfrac{n_c}{n}\sum_{j\in\pi} L_j\Big)\cdot\mathbb{I}(\pi\subseteq\mathcal{U}) = \tfrac{q}{pn_c}\sum_{\pi\in\Pi}\bar{L}_j\cdot\mathbb{I}(\pi\subseteq\mathcal{U}).$$

Since these indicator random variables are sampled in Stage 1 according to a $\mathrm{CRD}(pn_c/q, n_c)$ distribution, we may apply Lemma 4.5 to conclude that

$$\operatorname{Var}\Big(\mathop{\mathbb{E}}_{\mathbf{z}|\mathcal{U}}\big[\widehat{\mathrm{TTE}}_{\mathrm{PI}}\big]\Big) = \tfrac{1-(p/q)}{(p/q)(n_c-1)}\cdot\operatorname*{\widehat{Var}}_{\pi\in\Pi}\big(\bar{L}_\pi\big) = \tfrac{q-p}{p(n_c-1)}\cdot\operatorname*{\widehat{Var}}_{\pi\in\Pi}\big(\bar{L}_\pi\big).$$

Putting this together, we find that

$$\operatorname{Var}\Big(\widehat{\mathrm{TTE}}\Big) = \tfrac{1-q}{np-q}\cdot\operatorname*{\widehat{Var}}_{j\in[n]}\big(L_j\big) + \tfrac{(p-q)(1-np)}{p(np-q)(n_c-1)}\cdot\operatorname*{\widehat{Var}}_{\pi\in\Pi}\big(\bar{L}_\pi\big).$$

$\square$

B Experiment Details

B.1 Potential Outcomes Model

We generate synthetic potential outcomes based on a generalization of the response model from Ugander and Yin (2023) to incorporate β-order interactions:

$$Y_i(\mathbf{z}) = Y_i(\mathbf{0}) \cdot \left(1 + \delta z_i + \sum_{k=1}^{\beta} \gamma_k \cdot \binom{d_i}{k}^{-1} \sum_{\substack{\mathcal{S} \in \mathcal{S}_i^\beta \\ |\mathcal{S}|=k}} \prod_{j \in \mathcal{S}} z_j \right), \qquad Y_i(\mathbf{0}) = \left(a + b \cdot h_i + \varepsilon_i\right) \cdot \tfrac{d_i}{\overline{d}}.$$

In this model:

- a is a baseline effect. We select $a = 1$.
- $\mathbf{h} \in \mathbb{R}^n$ is a Fiedler vector of the graph Laplacian of the network which has undergone an affine transformation so that $\min(\mathbf{h}) = -1$ and $\max(\mathbf{h}) = 1$. This models network homophily effects.
- b controls the magnitude of the homophily effect. We select $b = 0$. We also ran the experiments with $b = 0.5$, to compare no homophily with some homophily, but the analysis and conclusions do not change. These are included later in the appendix.
- $\varepsilon_i \underset{\text{iid}}{\sim} N(0, \sigma)$ is a random perturbation of the baseline effect. We select $\sigma = 0.1$.
- d_i is the in-degree of vertex i. $\overline{d}$ is the average in-degree.
- δ is uniform direct effect on treated individuals. We select $\delta = 0.5$.
- γ_k is the effect of treated subsets of size k. We select $\gamma_k = 0.5^{k-1}$, which models marginal effects that decay with the size of the treated set.

B.2 Details of Real-World Networks

Here, we provide more details of the three real-world data sets we use in our analysis. We include all the raw data files, cleaned data, and processing scripts in our provided source code. A summary of the datasets is given in the following table.

Dataset	Vertices	Edges	Degree	Features
EMAIL Leskovec et al. (2007b); Yin et al. (2017); Leskovec and Krevl (2014)	employees $n = 1,005$	correspondence directed $\lvert E\rvert = 25,571$	min: 1 max: 334 average: 25	department $\lvert F\rvert = 42$
BLOGCATALOG Rossi and Ahmed (2015); Tang and Liu (2009b,a)	bloggers $n = 10,312$	connections undirected $\lvert E\rvert = 333,983$	min: 1 max: 3,992 average: 65	interests $\lvert F\rvert = 39$
AMAZON Leskovec et al. (2007a); Leskovec and Krevl (2014)	products $n = 14,436$	co-purchases directed $\lvert E\rvert = 70,832$	min: 1 max: 247 average: 5	category $\lvert F\rvert = 13,591$

Email

The EMAIL dataset is publicly available at `https://snap.stanford.edu/data/email-Eu-core.html` and is licensed under the BSD license[1]. This dataset models the email communications between members of a European research institution. The $n = 1,005$ vertices of the network are (anonymized) institution members, and there is a directed edge from individual i to individual j if i has sent at least one email to individual j.

It has a minimum degree of 1, a maximum degree of 212, and an average degree of 25.8, and its degree distribution is visualized in Figure 5; the support of the histogram has been cropped to remove some large outliers. The largest weakly connected component in the network contains 986 vertices, and the largest strongly connected component contains 803 vertices.

[1]For more information, see `https://snap.stanford.edu/snap/license.html` and `https://groups.google.com/g/snap-datasets/c/52MRzGbMkFg/m/FIFy_6qOCAAJ`

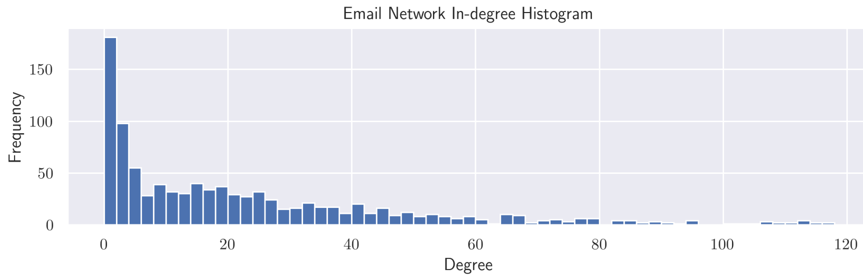


Figure 5: The degree distribution of the Email graph

Each individual in the network has been assigned one of 42 department labels. The sizes of these departments vary greatly, with the smallest department including a single individual and the largest department including 109 individuals. The average department size is 23.9. In the Email network, each vertex is assigned to exactly one department, and we use these assignments as our clustering. To pre-process this data for use in our experiments, we added self-loops to each node in the original dataset to represent the direct effect of the node's treatment on their outcome (See Section 2).

BlogCatalog

The BlogCatalog dataset is publicly available at https://networkrepository.com/soc-BlogCatalog-ASU.php and is licensed under a Creative Commons Attribution-ShareAlike License[2]. This dataset models the relationships between bloggers on the (now defunct) blogging website http://www.blogcatalog.com. The $n = 10,312$ nodes represent bloggers and the (undirected) edges represent the social network of the bloggers.

The network has a minimum degree of 1, a maximum degree of 3,992, and an average degree of 65, and its degree distribution is visualized in Figure 6; the support of the histogram has been cropped to remove some large outliers. The average clustering coefficient is approximately 0.46.

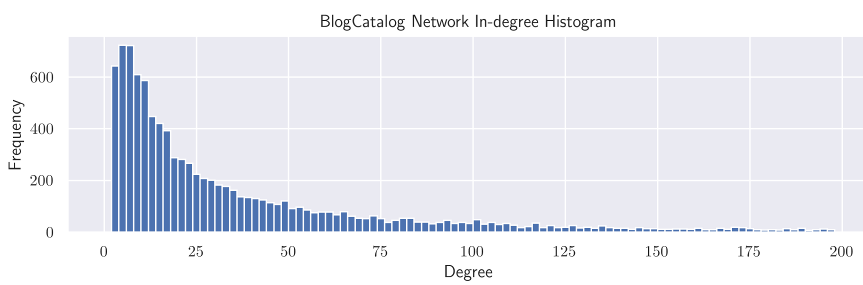


Figure 6: The degree distribution of the BlogCatalog graph

Each blogger in the network has an associated blog. Blogs (and thus, bloggers) are organized under interest categories specified by the website and can be listed under multiple categories. There are 39 such categories in this dataset and on average; on average, each blogger is listed under 1.6 categories. As part of the data pre-processing for our experiments, we added self-loops to each node in the original dataset, as we did with the Email dataset.

Amazon

The Amazon dataset is publicly available at https://snap.stanford.edu/data/amazon-meta.html and is licensed under the BSD license[3]. This dataset models an Amazon product co-purchasing network. The $n =$

[2] For more information, see https://networkrepository.com/policy.php

[3] For more information, see https://snap.stanford.edu/snap/license.html and https://groups.google.com/g/snap-datasets/c/52MRzGbMkFg/m/FIFy_6qOCAAJ

14, 436 nodes represent products and each node has outgoing edges to the top 5 products with which it is a frequent co-purchase. Thus, in addition to the self-loop at each node, each node has exactly 5 outgoing edges.

The network has a minimum in-degree of 1, a maximum in-degree of 247, and an average in-degree of 5; its in-degree distribution is visualized in Figure 7; the support of the histogram has been cropped to remove some large outliers.

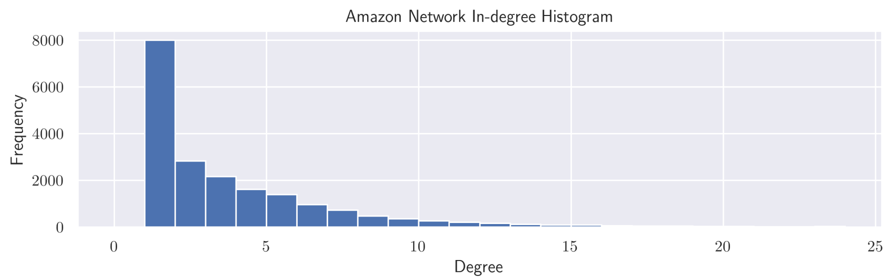


Figure 7: The degree distribution of the AMAZON graph

Products are organized into categories (which correspond to attributes such as the genre, setting, and actors in the film, as well as marketplace data such as the inclusion of these titles in certain deals or promotions) but can belong to multiple categories. There are 13,591 possible product categories; on average each product belongs to 13.2 categories. As part of the data pre-processing for our experiments, we added all self-loops and restricted the original dataset to only the product nodes labeled as DVDs.

B.3 Other Estimators

Here, we provide additional details of the other estimators used in our experiments Section 5.

Difference-in-Means

The difference-in-means (DM) approach estimates the total treatment effect as the difference in the average outcome of a treated individual and the average outcome of an untreated individual.

$$\widehat{\text{TTE}}_{\text{DM}} = \frac{\sum_i z_i \cdot Y_i(\mathbf{z})}{\sum_i z_i} - \frac{\sum_i (1-z_i) \cdot Y_i(\mathbf{z})}{\sum_i (1-z_i)}.$$

This estimator does not utilize any knowledge of the underlying graph. It only requires knowledge of the treatment assignments and the observed outcomes, which are always known to the experimenter. Under SUTVA, this is an unbiased estimator (since an individual's outcome is a function only of their treatment). However, it is not unbiased under interference; untreated individuals may have treated neighbors which impacts their outcome, introducing bias into our signal of the baseline effects. In general, in settings where the treatment effects are positive. This phenomenon outweighs the bias from untreated neighbors of treated individuals, so we observe a negative bias.

To counteract this bias, at the expense of requiring network knowledge, we can limit the set of individuals used in the estimator to those whose neighbors' treatment assignments largely align with theirs. We refer to this as a thresholded DM estimator.

Thresholded Difference-in-Means:

This family of estimators is parameterized by a value $\gamma \in [0, 1]$, which can be viewed as a stringency requirement that we place on the treatment assignments within one's neighborhood. In particular, we only include an individual in the "treated" set in this DM estimator if they are treated and at least a γ fraction of their neighbors are also treated. Similarly, we will only include an individual in the "untreated" set in this DM estimator if they are untreated and at most a $(1-\gamma)$ fraction of their neighbors are treated.

$$\widehat{\text{TTE}}_{\text{DM}(\gamma)} = \frac{\sum_i z_i \cdot Y_i(\mathbf{z}) \cdot \mathbb{I}\big(\sum_{j \in \mathcal{N}_i} z_i \geq \gamma d_i\big)}{\sum_i z_i \cdot \mathbb{I}\big(\sum_{j \in \mathcal{N}_i} z_i \geq \gamma d_i\big)} - \frac{\sum_i (1-z_i) \cdot Y_i(\mathbf{z}) \cdot \mathbb{I}\big(\sum_{j \in \mathcal{N}_i} z_i \leq (1-\gamma) d_i\big)}{\sum_i (1-z_i) \cdot \mathbb{I}\big(\sum_{j \in \mathcal{N}_i} z_i \leq (1-\gamma) d_i\big)}$$

Note that these estimators for $\gamma > 0$ require network knowledge to calculate the neighborhood treatment proportions, and they are biased under interference for the same reasoning as the standard DM estimator. Note that DM(0) (i.e., the thresholded DM estimator with parameter $\gamma = 0$) coincides with the ordinary DM estimator. The DM(1) estimator will only consider individuals with fully treated or untreated neighborhoods. As such, the DM(1) estimator will, under simpler randomization schemes like Bernoulli design, include very few individuals in its "treated" and "untreated" sets. The Horvitz-Thompson and Hájek estimators also exhibit this phenomenon.

Horvitz-Thompson:

The Horvitz-Thompson (HT) estimator (Horvitz and Thompson, 1952) uses inverse probability weighting to construct an unbiased TTE estimator under *arbitrary* potential outcomes models. To do this, it must only incorporate the outcomes from an individual's neighborhoods that are either fully treated or fully untreated, as these are the only outcomes that appear in the TTE estimand. The estimator has the form,

$$\begin{aligned}\widehat{\text{TTE}}_{\text{HT}} &= \tfrac{1}{n}\sum_{i\in[n]} \frac{Y_i(\mathbf{z})\cdot \mathbb{I}(\mathcal{N}_i \text{ fully treated})}{\Pr(\mathcal{N}_i \text{ fully treated})} - \tfrac{1}{n}\sum_{i\in[n]} \frac{Y_i(\mathbf{z})\cdot \mathbb{I}(\mathcal{N}_i \text{ fully untreated})}{\Pr(\mathcal{N}_i \text{ fully untreated})} \\ &= \tfrac{1}{n}\sum_{i\in[n]} \left[\frac{Y_i(\mathbf{z})\cdot\prod_{j\in\mathcal{N}_i} z_j}{\Pr\left(\prod_{j\in\mathcal{N}_i} z_j = 1\right)} - \frac{Y_i(\mathbf{z})\cdot\prod_{j\in\mathcal{N}_i}(1-z_j)}{\Pr\left(\prod_{j\in\mathcal{N}_i}(1-z_j)=1\right)} \right]\end{aligned}$$

From the first line, it is apparent that this estimator is unbiased. However, it relies on network knowledge to compute the exposure probabilities in the denominators of each fraction. A related inverse probability weighted estimator is the Hájek estimator.

Hájek

Since the HT estimator only considers individuals with fully treated and fully untreated neighborhoods, most of the bracketed terms within its summation will be 0. To compensate for this, we can adjust the $1/n$ normalization on the summation to use the expected number of non-zero entries corresponding to both terms in the bracketed expression. This change gives the Hájek estimator (Basu, 2011).

$$\widehat{\text{TTE}}_{\text{Hájek}} = \frac{\sum\limits_{i\in[n]} \frac{Y_i(\mathbf{z})\cdot\prod_{j\in\mathcal{N}_i} z_j}{\Pr\left(\prod_{j\in\mathcal{N}_i} z_j=1\right)}}{\sum\limits_{i\in[n]} \frac{\prod_{j\in\mathcal{N}_i} z_j}{\Pr\left(\prod_{j\in\mathcal{N}_i} z_j=1\right)}} - \frac{\sum\limits_{i\in[n]} \frac{Y_i(\mathbf{z})\cdot\prod_{j\in\mathcal{N}_i}(1-z_j)}{\Pr\left(\prod_{j\in\mathcal{N}_i}(1-z_j)=1\right)}}{\sum\limits_{i\in[n]} \frac{\prod_{j\in\mathcal{N}_i}(1-z_j)}{\Pr\left(\prod_{j\in\mathcal{N}_i}(1-z_j)=1\right)}}$$

The Hájek estimator trades off a reduction in the variance over the HT estimator for the introduction of some bias (a thorough discussion of this tradeoff is given by Khan and Ugander (2023)). As with the Horvitz-Thompson estimator, the calculation of exposure probabilities in this estimator requires knowledge of the interference network.

Two-Stage Estimator when $q = 1$

The one-stage estimator from Cortez et al. (2022) is

$$\widehat{\text{TTE}}^{\beta}_{\text{1-Stage}} := \frac{1}{n}\sum_{i=1}^{n}\sum_{t=0}^{\beta}\Big(\ell_{t,p}(1) - \ell_{t,p}(0)\Big)\cdot Y_i(\mathbf{z}^t), \quad \ell_{t,p}(x) = \prod_{\substack{s=0\\ s\neq t}}^{\beta} \tfrac{\beta x - ps}{pt - ps}. \tag{B.1}$$

When evaluating the estimator with $\beta = 1$, the estimator is simply

$$\widehat{\text{TTE}}^{\beta=1}_{\text{1-Stage}} = \frac{1}{np}\sum_{i=1}^{n}\Big(Y_i(\mathbf{z}^1) - Y_i(\mathbf{z}^0)\Big) \tag{B.2}$$

In what follows, we show that the two-stage rollout estimator with $q = 1$ is equivalent to $\widehat{\text{TTE}}^{\beta=1}_{\text{1-Stage}}$.

Theorem B.1. *Under a Two-Stage Rollout Design with budget p and effective treatment budget $q = 1$, the two-stage estimator defined in equation (3.1) under a model with degree β is equivalent to the estimator defined in (B.2).*

Proof. Under a Two-Stage Rollout Design with $q = 1$, we have

$$h_{t,q} = h_{t,1} = \prod_{\substack{s=0 \\ s\neq t}}^{\beta} \tfrac{\beta-s}{t-s} \; - \; \prod_{\substack{s=0 \\ s\neq t}}^{\beta} \tfrac{-s}{t-s}.$$

Notice that when $t \in \{1, 2, \ldots, \beta-1\}$, i.e. $t \neq 0$ and $t \neq \beta$, at some point we have a term corresponding to $s = 0$ and $s = \beta$ in the products above. Thus, both products are 0.

When $t = 0$, we have $h_{0,1} = \prod_{s=1}^{\beta} \frac{\beta-s}{0-s} - \prod_{s=1}^{\beta} \frac{-s}{0-s} = \prod_{s=1}^{\beta} \frac{\beta-s}{-s} - 1 = -1$ because the product equals 0 due to the $s = \beta$ term. Similarly, when $t = \beta$, we have $h_{\beta,1} = \prod_{s=0}^{\beta-1} \frac{\beta-s}{\beta-s} - \prod_{s=0}^{\beta-1} \frac{-s}{\beta-s} = 1$ since the second product will equal 0 due to the $s = 0$ term. To summarize, we have

$$h_{t,q} = \begin{cases} -1 & t = 0 \\ 0 & 1 \leq t \leq \beta - 1 \\ 1 & t = \beta \end{cases}.$$

□

B.4 Additional Experiments: Comparing Different Estimators

In this section, we have figures showing the MSE of different estimators as we vary the treatment budget p from 0.1 to 0.5 for different model degrees β and different real-world networks. As a reminder, we compare the following estimators:

- The two-stage polynomial interpolation estimator with $q = 0.5$ and no clustering, `2-Stage`
- The two-stage polynomial interpolation estimator with $q = 1$ and no clustering, `q=1`
- The one-stage polynomial interpolation estimator, `PI`
- The simple difference-in-means estimator, `DM`
- The thresholded difference-in-means estimator with parameter 0.75, `DM(0.75)`
- The Hájek estimator, `Hájek`

The first three estimators in this list are based on polynomial interpolation (PI), so we refer to them as the PI estimators. We refer to the others as the non-PI estimators. In all MSE plots, the lines indicate the empirical MSE over 1000 replications. In all bias and standard deviation plots, the bold line indicates the mean over 1000 replications, and the shading indicates the experimental standard deviation, calculated by taking the square root of the experimental variance over all replications.

In Figure 8, we show the MSE corresponding to Figure 2 from Section 5. The column faceting indicates model degree; note that the y-axis limits differ across these subplots. When $\beta = 1$, `PI` and `q=1` are equivalent and have slightly lower MSE compared with `2-Stage`. However, the difference is hard to see without zooming in further since the lines almost overlap. Note that the difference-in-means estimators have MSE outside the bounds of the plots. When $\beta = 2$, the results are similar but you can start to see the difference between the three PI estimators, which all have lower MSE when compared with the non-PI estimators. For smaller values of p, the estimator `PI` has slightly lower MSE, followed by `2-Stage`, followed by `q=1`. Again, the difference is quite small. In this case, as noted in the main body of the paper, we are in a setting where using the one-stage rollout and estimator is preferable. When $\beta = 3$, the difference between the three PI estimators is more pronounced. The `2-Stage` has the lowest MSE, especially for lower values of p. The `q=1` estimator has MSE relatively close to it for all p-values, but does slightly worse, although better than `PI` for small p values. In this case, we have a setting where the two-stage approach is valuable as it outperforms the other methods.

In Figure 9, we show the MSE and the bias and standard deviation of the different estimators under the BlogCatalog network. We omit the `Hájek` estimator because the network degree is very high; under unit randomization, the estimator is often undefined. In all cases, the two difference-in-means estimators are very biased, so their MSE is much worse than the PI estimators. Similar to the Amazon network, when $\beta = 1$ the PI estimators are almost indistinguishable, with `2-Stage` coming in with slightly higher MSE due to a small

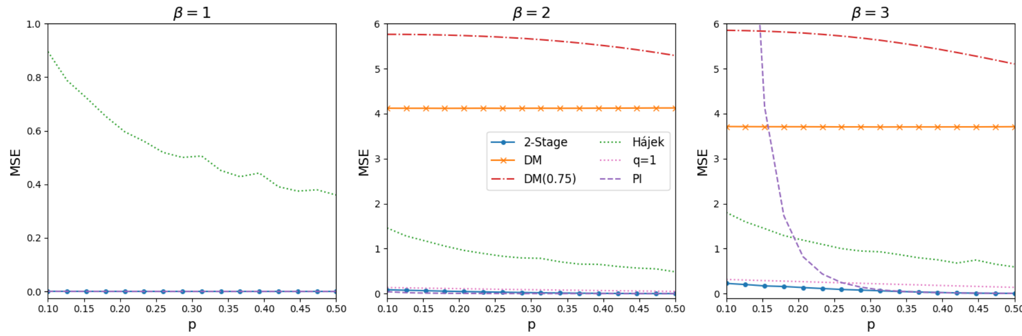


Figure 8: AMAZON Network. MSE of different estimators as a function of treatment budget p.

increase in variance. The difference-in-means estimators do not appear on the plot since their MSE exceeds the plotting range. When $\beta = 2$, we see that `PI` has higher MSE for smaller values of p due to an increased variance (the estimator is unbiased). `2-Stage` has much lower variance than `PI` and its bias decreases as p approaches 0.5. `q=1` has even lower variance than `2-Stage` and similar bias, but its bias remains worse than `2-Stage`. However, their MSE remains comparable. When $\beta = 3$, there is a much clearer difference between the PI estimators. For most values of p, `PI` has the worst variance (due to extrapolation with a richer model), while `q=1` has the worst bias (due to the heavier reliance on the subsampling). Meanwhile, `2-Stage` is in between, with lower bias, but larger variance than `q=1` and with higher bias, but lower variance than `PI`. In terms of MSE, `q=1` outperforms the other estimators. Recall that the `q=1` estimator is equivalent to the $\beta = 1$ version of the one-stage PI estimator. This setting shows that although the two-stage approach can greatly reduce error over the one-stage approach even without clustering, an even simpler design (one-stage rollout over just two time steps) and estimator (using observations from the two time steps) can still outperform.

The results from Figure 10 are the same as Figure 9.

B.5 Additional Experiments: Comparing Different Clusterings

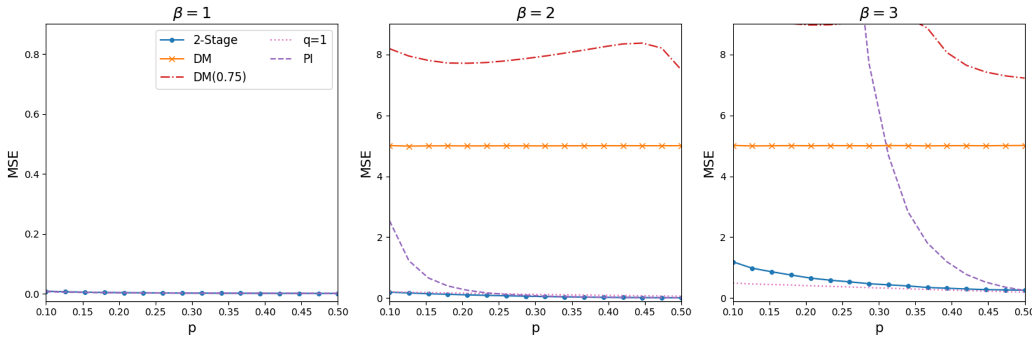
We compare the performance of the `2-Stage` estimator under two clustering methods versus no clustering in the first stage of the experimental design. In the **clustering with full graph knowledge**, we cluster the true underlying graph using the METIS clustering library Karypis and Kumar (1998). In the **clustering with covariate knowledge**, clusters are based on features. When each vertex is assigned to one feature, we use these assignments as the clustering. When vertices may have multiple features we form a feature graph — a weighted graph, where the weight of edge (i, j) is the number of feature labels shared by i and j — and cluster this feature graph using METIS. In all plots, the column faceting indicates the type of clustering and the y-axis varies q on the interval $[p, 1]$, where $p = 1$.

We also include tables with various pieces of information pertaining to the performance of the two-stage design and estimator, including clustering metrics such as number of cut edges, the cut effect $C(\delta(\Pi))$, and the empirical variance across clusters of cluster average influences $\widehat{\mathrm{Var}}(\bar{L}_\pi)$. The latter two metrics are defined in Section 3. In each row, $q_{\min}$ is the value of q that minimizes the MSE and the column $\mathrm{MSE}(q_{\min})$ contains that value.

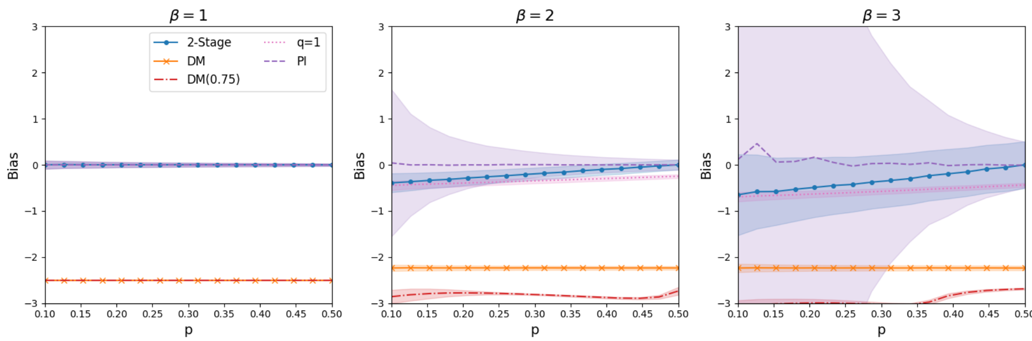
Table 4: Clustering Metrics for BLOGCATALOG Network

β	Cluster	$\widehat{\mathrm{Var}}(\bar{L}_\pi)$	$C(\delta(\Pi))$	Cut Edges	$q_{\min}$	$\mathrm{MSE}(q_{\min})$
2	Full	0.697	0.471	604504	0.5	0.260
2	Covariate	0.059	0.486	643080	0.5	0.190
3	Full	0.703	0.717	604504	1	0.610
3	Covariate	0.060	0.734	643080	1	0.486

In Figure 11, we show the results for the BLOGCATALOG network under a model with degree $\beta = 2$. In this case, the clusterings each have $n_c = 50$ clusters. For this network, clustering does not appear to be of any help in reducing the bias and at worst, under a clustering that uses full graph knowledge, increases variance. Taking a look at the first two rows of Table 4 sheds some light on this. We see that the $\widehat{\mathrm{Var}}(\bar{L}_\pi)$ under a clustering that



(a) MSE of different estimators as a function of treatment budget p.



(b) Bias and variance of different estimators as a function of treatment budget p.

Figure 9: BlogCatalog Network.

uses full graph knowledge is more than ten times higher than a clustering that only uses covariate information. The number of cut edges is similar under both clusterings and thus so is the cut effect. In this example, it would appear that one is better off not clustering at all.

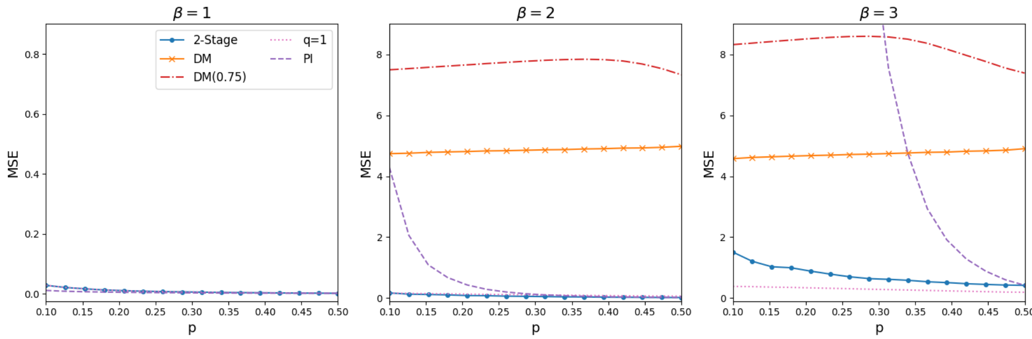
In Figure 12, we show the results for the Email network under a model with degree $\beta = 2$. In this case, the clusterings each have $n_c = 42$ clusters. We see an advantage with clustering on covariates in particular. The highest bias, but lowest variance, is under no clustering. The clustering with full knowledge certainly decreases variance versus no clustering, but at the expense of incurring a lot of variance. The lowest MSE is achieved by the covariate knowledge clustering at $q = 1$, which strikes a balance between bias and variance. Taking a look at Table 5, we see that the $\widehat{\text{Var}}(\bar{L}_\pi)$ term is similar under both clusterings. However, the covariate clustering cuts about a quarter less edges than the full knowledge clustering and thus has a smaller cut effect.

Table 5: Clustering Metrics for Email Network

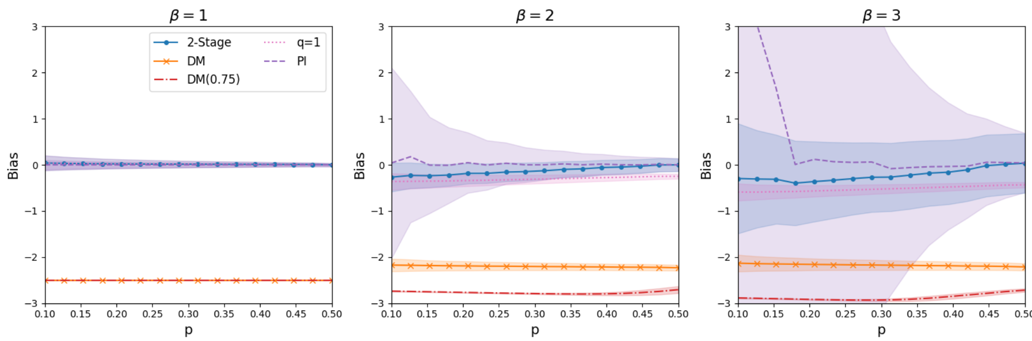
β	Cluster	$\widehat{\text{Var}}(\bar{L}_\pi)$	$C(\delta(\Pi))$	Cut Edges	$q_{\min}$	MSE($q_{\min}$)
2	Full	0.399	0.442	21756	0.5	0.232
2	Covariate	0.398	0.372	16284	1	0.133
3	Full	0.417	0.686	21756	1	0.483
3	Covariate	0.412	0.591	16284	1	0.288

B.6 Additional Experiments: Homophily Parameter $b = 0.5$.

In this section, we show some results when the model exhibits homophily by setting the parameter $b = 0.5$. All other parameters are set to the same values as previous plots. Although there are some small visual differences between the plots in this section and the plots throughout the rest of this work, the analyses and conclusions remain the same. For example, we can compare Figure 8 (where $b = 0$) with 13a (where $b = 0.5$). Both of these show the MSE of different estimators for different values of treatment budgets p and different model degrees β. Notice the difference in the scaling on the y-axis, particularly for $\beta = 2$ and $\beta = 3$. However, the patterns are the same: for most values of p, the two difference in means estimators have the highest MSE, followed by the Hájek



(a) MSE of different estimators as a function of treatment budget p.



(b) Bias and variance of different estimators as a function of treatment budget p.

Figure 10: Email Network.

estimator, and then followed by the three PI estimators. When $\beta = 3$, the MSE of the vanilla PI estimator is extremely high for small values of p, but gets smaller than the non-PI estimators around $p = 0.2$. In general, for $\beta = 3$, `2-Stage` tends to outperform `PI` for many paramter values and for some networks, `q=1` has the smallest MSE in some cases. When $\beta = 2$, we see that the two stage approach improves over the one stage approach under the BlogCatalog and Email networks for small values of p. When $\beta = 1$ the performances of the PI estimators are similar, with `2-Stage` performing ever so slightly worse.

In Figure 14, we show the performance of the two stage approach under two different clustering versus no clustering for three different networks. The BlogCatalog and Email network results are very similar to those in Figures 11 and 12. The Amazon network result sheds some light onto why the scaling is different in the Amazon MSE plots: the bias has a larger magnitude. Part of this is likely attributable to the fact that switching from $b = 0$ to $b = 0.5$ changed the magnitude of the baseline outcomes, and therefore all outcomes.

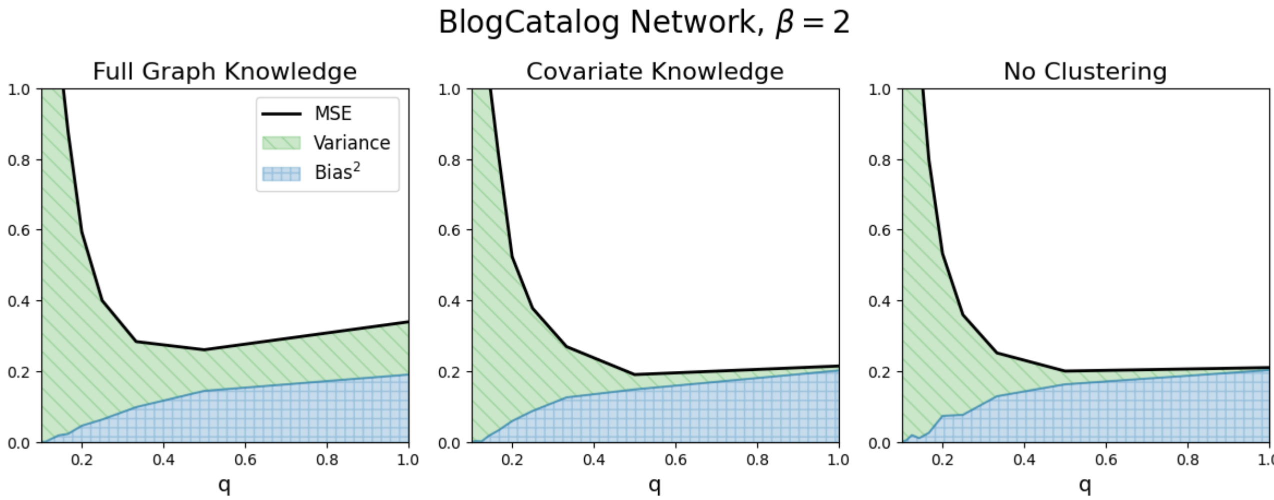


Figure 11: BlogCatalog Network. MSE of `2-Stage` estimator under two different clusterings versus no clustering, as a function of q.

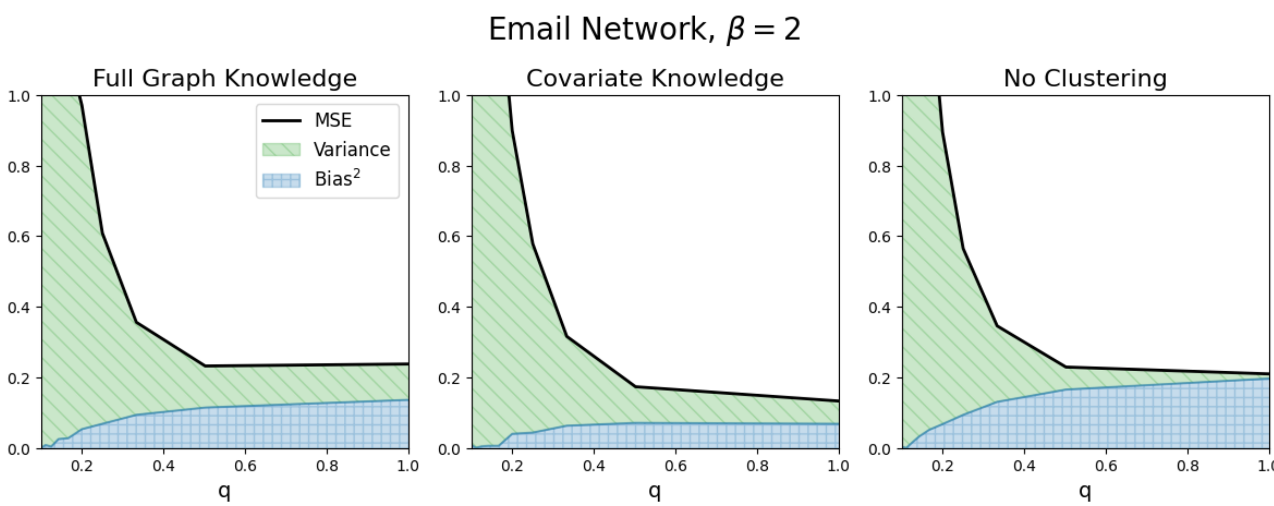
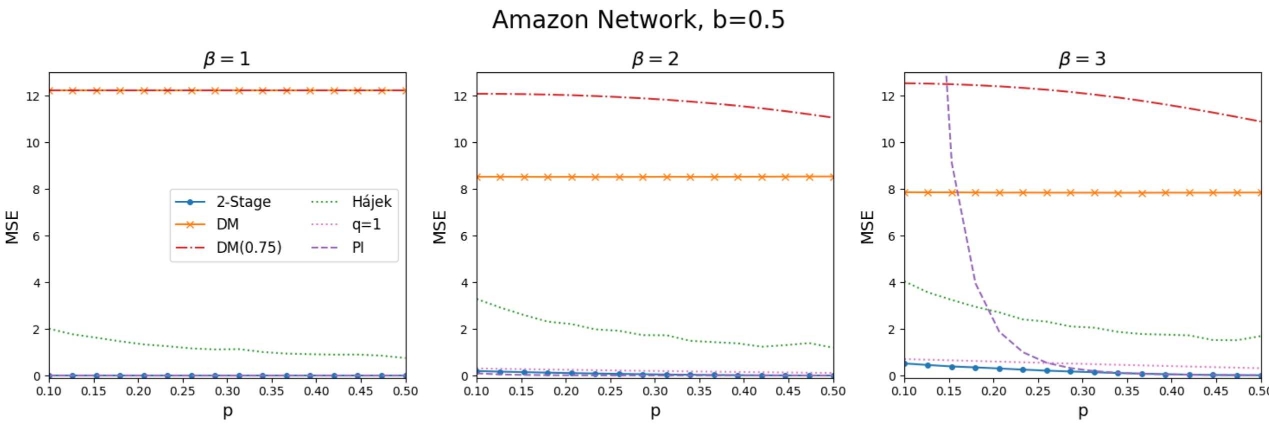
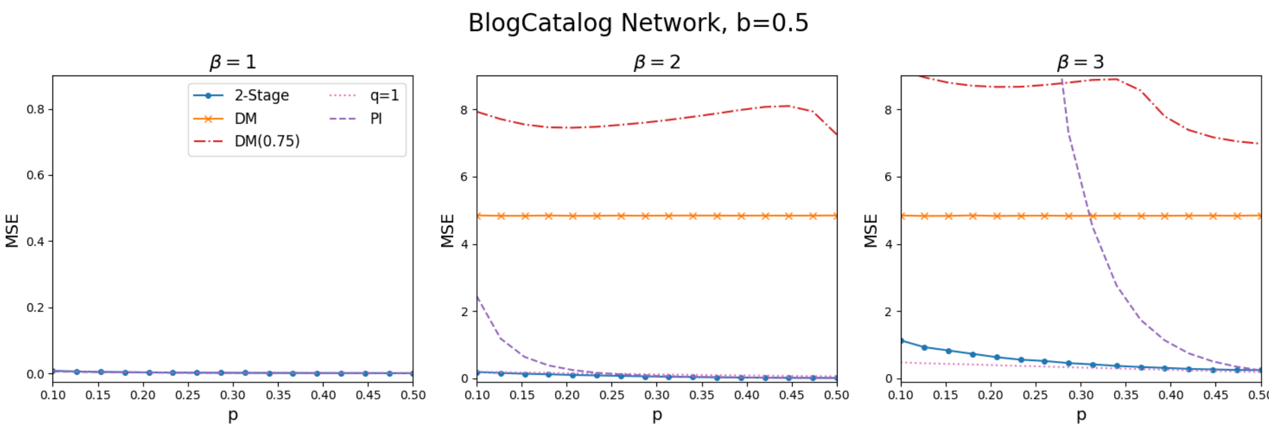


Figure 12: Email Network. MSE of `2-Stage` estimator under two different clusterings versus no clustering, as a function of q.



(a)



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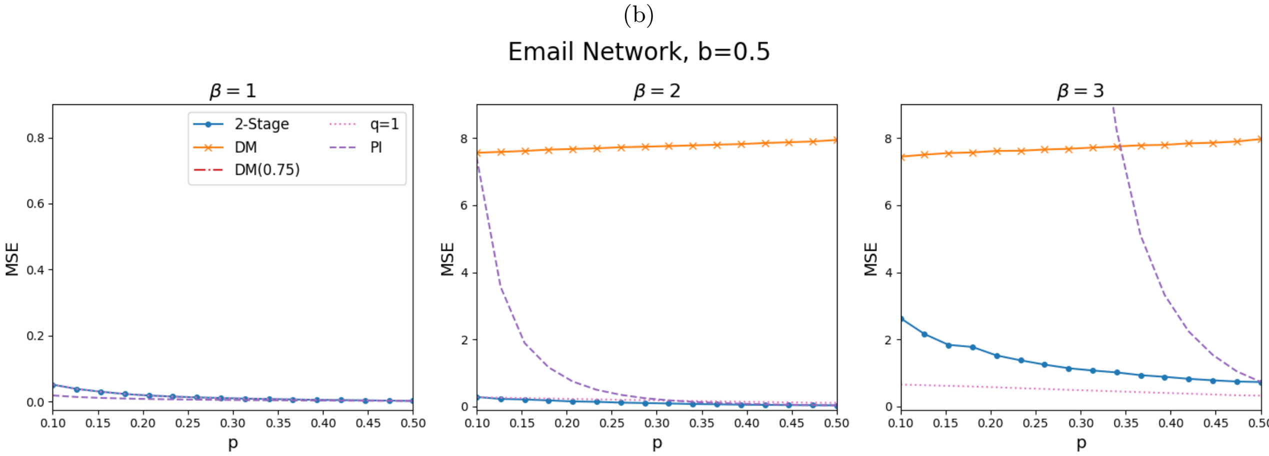
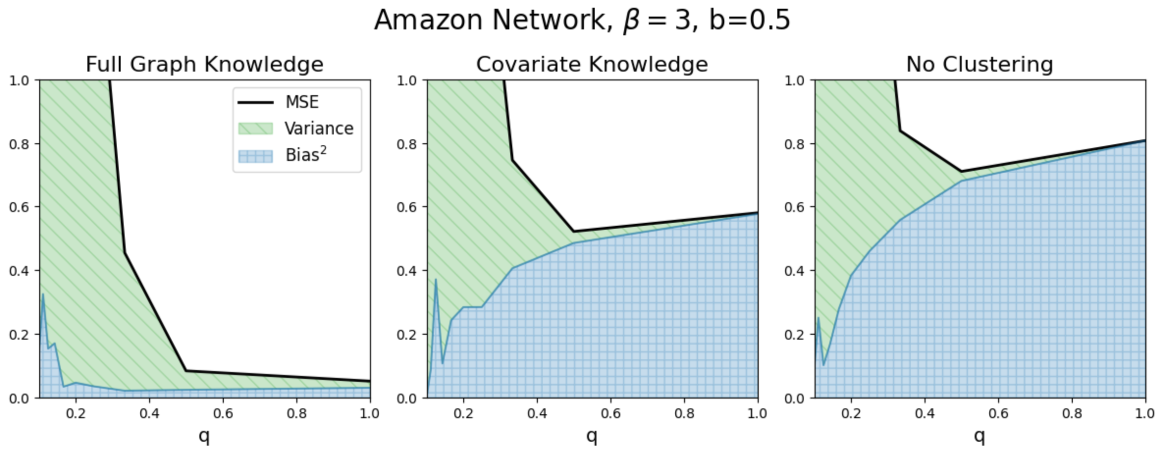


(c)

Figure 13



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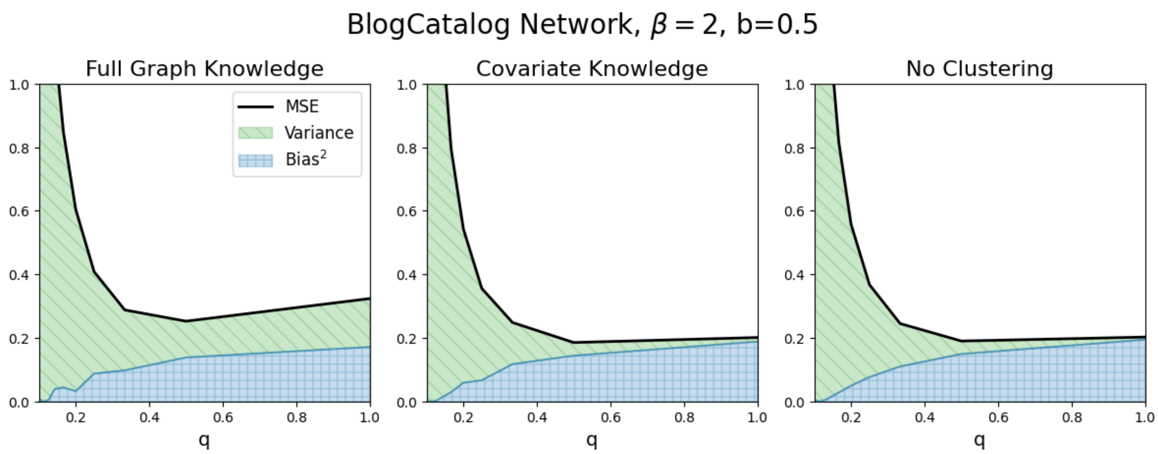

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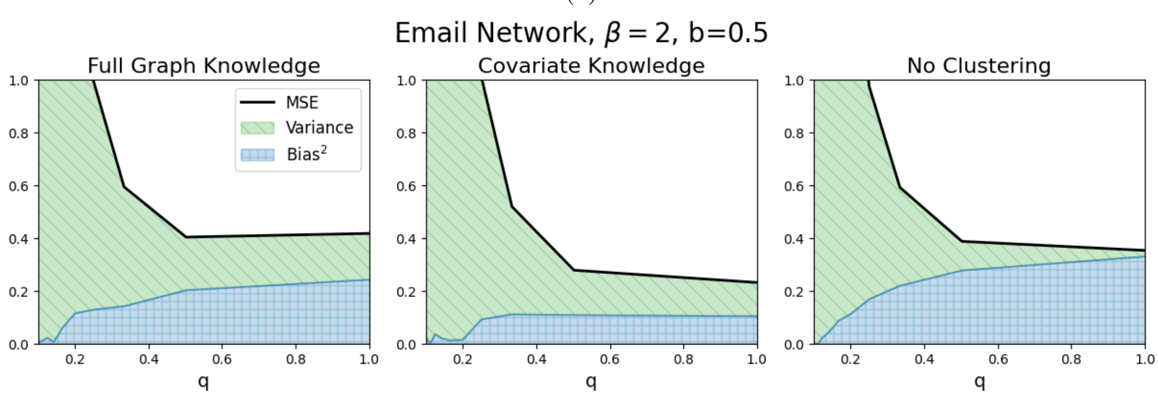

(c)

Figure 14