A Mathematical Appendix: Proofs of Theorems

A.1 Lemmas

Below, we describe all the lemmas, which are used to prove the main theorems of this paper. For completeness, their proofs appear in the supplementary appendix.

LEMMA 1 (AN ALTERNATIVE DEFINITION OF THE K-WAY AVERAGE INTERACTION EFFECT) *The K-way average interaction effect (AIE) of treatment combination $\mathbf{T}_i^{1:K} = \mathbf{t}^{1:K} = (t_1, \ldots, t_K)$ relative to baseline condition $\mathbf{T}_i^{1:K} = \mathbf{t}_0^{1:K} = (t_{01}, \ldots, t_{0K})$, given in Definition 3, can be rewritten as,*

$$\xi_{1:K}(\mathbf{t}^{1:K}; \mathbf{t}_0^{1:K}) \;=\; \xi_{1:(K-1)}(\mathbf{t}^{1:(K-1)}; \mathbf{t}_0^{1:(K-1)} \mid T_{iK} = t_K) - \xi_{1:(K-1)}(\mathbf{t}^{1:(K-1)}; \mathbf{t}_0^{1:(K-1)} \mid T_{iK} = t_{0K}).$$

LEMMA 2 *Under Assumption 2, for any $k = 1, \ldots, K$, the following equality holds,*

$$\begin{aligned}\int_{\overline{\mathcal{F}}^{\mathcal{K}_k}} \xi_{\mathcal{K}_K}(\tilde{\mathbf{T}}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_K}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k}) \;&=\; \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\ &+ \sum_{\ell=1}^{k} (-1)^{\ell} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \int_{\overline{\mathcal{F}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}).\end{aligned}$$

LEMMA 3 (DECOMPOSITION OF THE K-WAY AIE) *The K-way Average Treatment Interaction Effect (AIE) (Definition 3), can be decomposed into the sum of the K-way conditional Average Treatment Combination Effects (ACEs). Formally, let $\mathcal{K}_k \subseteq \mathcal{K}_K = \{1, \ldots, K\}$ with $|\mathcal{K}_k| = k$ where $k = 1, \ldots, K$. Then, the K-way AIE can be written as follows,*

$$\xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K}) \;=\; \sum_{k=1}^{K} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}),$$

where the second summation is taken over the set of all possible $\mathcal{K}_k$ and the k-way conditional ACE is defined as,

$$\tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \;=\; \mathbb{E}\left\{ \int_{\underline{\mathcal{F}}^{\mathcal{K}_K}} \{Y_i(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}, \underline{T_i}^{\mathcal{K}_K}) - Y_i(\mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}, \underline{T_i}^{\mathcal{K}_K})\} dF(\underline{\mathbf{T}}_i^{\mathcal{K}_K}) \right\}$$

LEMMA 4 (DECOMPOSITION OF THE K-WAY AMIE) *The K-way Average Marginal Treatment Interaction Effect (AMIE), defined in Definition 2, can be decomposed into the sum of the K-way Average Treatment Combination Effects (ACEs). Formally, let*

$\mathcal{K}_k \subseteq \mathcal{K}_K = \{1, \dots, K\}$ *with* $|\mathcal{K}_k| = k$ *where* $k = 1, \dots, K$. *Then, the* K*-way AMIE can be written as follows,*

$$\pi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K}) \;=\; \sum_{k=1}^{K} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k}),$$

where the second summation is taken over the set of all possible $\mathcal{K}_k$.

A.2 Proof of Theorem 1

We use proof by induction. Under Assumption 2, we first show for $K = 2$. To simplify the notation, we do not write out the $J-2$ factors that we marginalize out. We begin by decomposing the AME as follows,

$$\begin{aligned}
\psi_A(a_l, a_0) \;&=\; \int_{\mathcal{B}} \mathbb{E}\{Y_i(a_\ell, B_i) - Y_i(a_0, B_i)\} \; dF(B_i) \\
&= \mathbb{E}\{Y_i(a_\ell, b_0) - Y_i(a_0, b_0)\} + \int_{\mathcal{B}} \mathbb{E}\{Y_i(a_\ell, B_i) - Y_i(a_0, B_i) - Y_i(a_\ell, b_0) + Y_i(a_0, b_0)\} \; dF(B_i) \\
&= \mathbb{E}\{Y_i(a_\ell, b_0) - Y_i(a_0, b_0)\} + \int_{\mathcal{B}} \xi_{AB}(a_\ell, B_i; a_0, b_0) \; dF(B_i).
\end{aligned}$$

Similarly, we have $\psi_B(b_m, b_0) = \mathbb{E}\{Y_i(a_0, b_m) - Y_i(a_0, b_0)\} + \int_{\mathcal{A}} \xi_{AB}(A_i, b_m; a_0, b_0) \; dF(A_i)$. Given the definition of the AMIE in equation (5), we have,

$$\begin{aligned}
\pi_{AB}(a_\ell, b_m, a_0, b_0) \;&=\; \mathbb{E}\{Y_i(a_\ell, b_m) - Y_i(a_0, b_0)\} - \psi_A(a_\ell, a_0) - \psi_B(b_m, b_0) \\
= \xi_{AB}(a_\ell, b_m; a_0, b_0) &- \int_{\mathcal{B}} \xi_{AB}(a_\ell, B_i; a_0, b_0) \; dF(B_i) - \int_{\mathcal{A}} \xi_{AB}(A_i, b_m; a_0, b_0) \; dF(A_i).
\end{aligned}$$

This proves that the AMIE is a linear function of the AIEs. We next show that the AIE is also a linear function of the AMIEs.

$$\begin{aligned}
\xi_{AB}(a_\ell, b_m; a_0, b_0) \;&= \mathbb{E}[Y_i(a_\ell, b_m) - Y_i(a_0, b_0)] - \psi_A(a_\ell, a_0) - \psi_A(b_m, b_0) \\
&\quad - \mathbb{E}[Y_i(a_\ell, b_0) - Y_i(a_0, b_0)] + \psi_A(a_\ell, a_0) - \mathbb{E}[Y_i(a_0, b_m) - Y_i(a_0, b_0)] + \psi_A(b_m, b_0) \\
&= \pi_{AB}(a_\ell, b_m; a_0, b_0) - \pi_{AB}(a_\ell, b_0; a_0, b_0) - \pi_{AB}(a_0, b_m; a_0, b_0).
\end{aligned}$$

Thus, we obtain the desired results for $K = 2$.

Now we show that if the theorem holds for any K with $K \geq 2$, it also holds for $K+1$. First, using Lemma 2, we rewrite the equation of interest as follows,

$$\pi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K}) = \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K}) + \sum_{k=1}^{K-1}(-1)^k \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \left\{ \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \right.$$
$$\left. + \sum_{\ell=1}^{k}(-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \int_{\overline{\mathcal{F}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}) \right\}.$$

Utilizing the the definition of the K-way AMIE given in Definition 2 and the assumption that the theorem holds for K, we have,

$$\pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) = \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) - \sum_{k=1}^{K} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \pi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k})$$
$$= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}})$$
$$- \sum_{k=1}^{K} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \left[\xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k}) + \sum_{m=1}^{k-1}(-1)^m \sum_{\mathcal{K}_m \subseteq \mathcal{K}_k} \left\{ \xi_{\mathcal{K}_k \setminus \mathcal{K}_m}(\mathbf{t}^{\mathcal{K}_k \setminus \mathcal{K}_m}, \mathbf{t}_0^{\mathcal{K}_k \setminus \mathcal{K}_m}) \right. \right.$$
$$\left. \left. + \sum_{\ell=1}^{m}(-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_m} \int_{\overline{\mathcal{F}}^{\mathcal{K}_m \setminus \mathcal{K}_\ell}} \xi_{\mathcal{K}_k \setminus \mathcal{K}_m}(\mathbf{t}^{\mathcal{K}_k \setminus \mathcal{K}_m}, \mathbf{t}_0^{\mathcal{K}_k \setminus \mathcal{K}_m} \mid \tilde{\mathbf{T}}^{\mathcal{K}_m \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_m \setminus \mathcal{K}_\ell}) \right\} \right]. \tag{17}$$

After rearranging equation (17), the coefficient for $\xi_{\mathcal{K}_{K+1} \setminus \mathcal{K}_u}(\mathbf{t}^{\mathcal{K}_{K+1} \setminus \mathcal{K}_u}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_u})$ is equal to $(-1)^u$. Similarly, the coefficient of the following term is equal to $(-1)^{u+v}$.

$$\int_{\overline{\mathcal{F}}^{\mathcal{K}_u \setminus \mathcal{K}_v}} \xi_{\mathcal{K}_{K+1} \setminus \mathcal{K}_u}(\mathbf{t}^{\mathcal{K}_{K+1} \setminus \mathcal{K}_u}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_u} \mid \tilde{\mathbf{T}}^{\mathcal{K}_u \setminus \mathcal{K}_v}, \overline{\mathbf{T}}_i^{\mathcal{K}_v} = \mathbf{t}_0^{\mathcal{K}_v}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_u \setminus \mathcal{K}_v}).$$

Therefore, we can rewrite equation (17) as follows,

$$\pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}})$$
$$= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) + \sum_{k=1}^{K}(-1)^k \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \left[\xi_{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}) \right.$$
$$\left. + \sum_{\ell=1}^{k-1}(-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \int_{\overline{\mathcal{F}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}} \xi_{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}) \right]$$
$$= \xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) + \sum_{k=1}^{K}(-1)^k \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \left[\xi_{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}) \right.$$
$$\left. + \sum_{\ell=1}^{k}(-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \int_{\overline{\mathcal{F}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}} \xi_{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}) \right]$$

$$= \xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) + \sum_{k=1}^{K}(-1)^k \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \int \xi(\mathbf{T}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) dF(\mathbf{T}^{\mathcal{K}_k}),$$

where the second equality follows from applying Lemma 1 to $\tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}})$ and the final equality from Lemma 2. This proves that the K-way AMIE is a linear function of the K-way AIEs.

We next prove that the K-way AIE can be written as a linear function of the K-way AMIEs. We will show this by mathematical induction. We already show the desired result holds for $K = 2$. Choose any $K \geq 2$ and assume that the following equality holds,

$$\xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K}) \;=\; \sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}).$$

Using the definition of the K-way AIE given in Lemma 1, we have

$$\begin{aligned}
\xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) \;&=\; \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K} \mid T_i^{K+1} = t^{K+1}) - \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K} \mid T_i^{K+1} = t_0^{K+1}) \\
= \sum_{k=1}^{K}(-1)^{K-k} &\sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t^{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t^{K+1}) \\
- \sum_{k=1}^{K}(-1)^{K-k} &\sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t_0^{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t_0^{K+1}),
\end{aligned}$$

where the second equality follows from the assumption. Let us consider the following decomposition.

$$\begin{aligned}
&\sum_{k=1}^{K+1}(-1)^{K-k+1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}) \\
= &\sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t^{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t_0^{K+1}) + (-1)^K \pi_{\mathcal{K}_{K+1}}(\mathbf{t}_0^{\mathcal{K}_K}, t^{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_0^{K+1}) \\
&+ \sum_{k=1}^{K}(-1)^{K-k+1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t_0^{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t_0^{K+1}), \qquad (18)
\end{aligned}$$

where the first and second terms together represent the cases with $K + 1 \in \mathcal{K}_k$, while the third term corresponds to the cases with $K + 1 \in \mathcal{K}_{K+1} \setminus \mathcal{K}_k$. Note that these two cases are mutually exclusive and exhaustive. Finally, note the following equality,

$$\sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t^{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k}, t^{K+1})$$

$$= \sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}, t^{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}, t_0^{K+1}) + (-1)^K \pi_{\mathcal{K}_{K+1}}(\mathbf{t}_0^{\mathcal{K}_K}, t^{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_0^{K+1}). \quad (19)$$

Then, together with equations (18) and (19), we obtain,

$$\xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) = \sum_{k=1}^{K+1}(-1)^{K-k+1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}).$$

Thus, the desired linear relationship holds for any $K \geq 2$. $\square$

A.3 Proof of Theorem 2

To prove the invariance of the K-way AMIE, note that Lemma 4 implies,

$$\pi_{\mathcal{K}_K}(\mathbf{t}; \mathbf{t}_0) - \pi_{\mathcal{K}_K}(\tilde{\mathbf{t}}; \mathbf{t}_0) = \sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \tilde{\mathbf{t}}^{\mathcal{K}_k}). \quad (20)$$

$$\pi_{\mathcal{K}_K}(\mathbf{t}; \tilde{\mathbf{t}}_0) - \pi_{\mathcal{K}_K}(\tilde{\mathbf{t}}; \tilde{\mathbf{t}}_0) = \sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \tilde{\mathbf{t}}^{\mathcal{K}_k}). \quad (21)$$

Thus, the K-way AMIE is interval invariant. To prove the lack of invariance of the K-way AIE, note that according to Lemma 3, we can rewrite equation (11) as follows.

$$\sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \left\{ \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) - \tau_{\mathcal{K}_k}(\tilde{\mathbf{t}}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \right\}$$
$$= \sum_{k=1}^{K}(-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \left\{ \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \tilde{\mathbf{t}}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) - \tau_{\mathcal{K}_k}(\tilde{\mathbf{t}}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \tilde{\mathbf{t}}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \right\}.$$

It is clear that this equality does not hold in general because the K-way conditional ACEs are conditioned on different treatment values. Thus, the K-way AIE is not interval invariant. $\square$

A.4 Proof of Theorem 3

We use L to denote the objective function in equation (12). Since it is a convex optimization problem, it has one unique solution and the solution should satisfy the following equalities.

$$\frac{\partial L}{\partial \mu} = 0, \qquad \frac{\partial L}{\partial \beta_\ell^j} = 0 \quad \text{for all } j, \text{ and } \ell \in \{0, 1, \ldots, L_j - 1\},$$

$$\frac{\partial L}{\partial \beta^{jj'}_{\ell,m}} \;=\; 0, \quad \text{for all } j \neq j',\ \ell \in \{0,1,\ldots,L_j-1\} \text{ and } m \in \{0,1,\ldots,L_{j'}-1\},$$
$$\frac{\partial L}{\partial \beta^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}}} \;=\; 0 \quad \text{for all } \mathbf{t}^{\mathcal{K}_k},\ \text{and } \mathcal{K}_k \subset \mathcal{K}_J \text{ such that } k \geq 3. \tag{22}$$

For the sake of simplicity, we introduce the following notation.

$$\mathcal{S}(\mathbf{t}^{\mathcal{K}_k}) \;\equiv\; \{i; \mathbf{T}_i^{\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_k}\}, \quad N_{\mathbf{t}^{\mathcal{K}_k}} \;\equiv\; \sum_{i=1}^{n} \mathbf{1}\{\mathbf{T}_i^{\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_k}\}, \quad \hat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_k}] \;\equiv\; \frac{1}{N_{\mathbf{t}^{\mathcal{K}_k}}} \sum_{i \in \mathcal{S}(\mathbf{t}^{\mathcal{K}_k})} Y_i.$$

Then, from $\frac{\partial L}{\partial \boldsymbol{\beta}^{\mathcal{K}_J}_{\mathbf{t}^{\mathcal{K}_J}}} = 0$ for all $\mathbf{t}^{\mathcal{K}_J}$,

$$\frac{\partial L}{\partial \boldsymbol{\beta}^{\mathcal{K}_J}_{\mathbf{t}^{\mathcal{K}_J}}} = \sum_{i \in \mathcal{S}(\mathbf{t}^{\mathcal{K}_k})} -2\Bigg(Y_i - \mu - \sum_{j=1}^{J}\sum_{\ell=0}^{L_j-1} \beta^j_\ell \mathbf{1}\{T_{ij}=\ell\} - \sum_{j=1}^{J-1}\sum_{j'>j}\sum_{\ell=0}^{L_j-1}\sum_{m=0}^{L_{j'}-1} \beta^{jj'}_{\ell m}\mathbf{1}\{T_{ij}=\ell, T_{ij'}=m\}$$
$$- \sum_{k=3}^{J}\sum_{\mathcal{K}_k\subset\mathcal{K}_J}\sum_{\mathbf{t}^{\mathcal{K}_k}} \beta^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}} \mathbf{1}\{\mathbf{T}_i^{\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_k}\}\Bigg) = 0. \tag{23}$$

Therefore, for all $\mathbf{t}^{\mathcal{K}_J}$,

$$\hat{\mu} + \sum_{k=1}^{J}\sum_{\mathcal{K}_k\subset\mathcal{K}_J}\sum_{\mathbf{t}^{\mathcal{K}_k}} \beta^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}} \mathbf{1}\{\mathbf{t}^{\mathcal{K}_k} \subset \mathbf{t}^{\mathcal{K}_J}\} \;=\; \widehat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_J} = \mathbf{t}^{\mathcal{K}_J}].$$

For the first-order effect, we can use the weighted zero-sum constraints for all factors except for the j th factor. In particular, for all j and $t_{j\ell} \in \mathbf{t}^{\mathcal{K}_J}$,

$$\sum_{j'\neq j}\sum_{\ell=0}^{L_{j'}-1}\prod_{t_{j'\ell}\in\mathbf{t}^{\mathcal{K}_J\setminus j}} \Pr(T_{ij'}=\ell)\Bigg\{\hat{\mu} + \sum_{k=1}^{J}\sum_{\mathcal{K}_k\subset\mathcal{K}_J}\sum_{\mathbf{t}^{\mathcal{K}_k}} \beta^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}}\mathbf{1}\{\mathbf{t}^{\mathcal{K}_k} \in \mathbf{t}^{\mathcal{K}_J}\}\Bigg\}$$
$$= \sum_{j'\neq j}\sum_{\ell=0}^{L_{j'}-1}\prod_{t_{j'\ell}\in\mathbf{t}^{\mathcal{K}_J\setminus j}} \Pr(T_{ij'}=\ell)\ \ \widehat{\mathbb{E}}[Y_i \mid T_{ij}=\ell, \mathbf{T}_i^{\mathcal{K}_J\setminus j} = \mathbf{t}^{\mathcal{K}_J\setminus j}]$$
$$\iff \hat{\beta}^j_\ell \;=\; \sum_{j'\neq j}\sum_{\ell=0}^{L_{j'}-1}\prod_{t_{j'\ell}\in\mathbf{t}^{\mathcal{K}_J\setminus j}} \Pr(T_{ij'}=\ell)\ \ \widehat{\mathbb{E}}[Y_i \mid T_{ij}=\ell, \mathbf{T}_i^{\mathcal{K}_J\setminus j} = \mathbf{t}^{\mathcal{K}_J\setminus j}] - \hat{\mu}.$$

In general, for all $\mathbf{t}^{\mathcal{K}_k}, \mathcal{K}_k \subset \mathcal{K}_J$ and $k \geq 2$,

$$\hat{\beta}^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}} = \sum_{j'\in\mathcal{K}_J\setminus\mathcal{K}_k}\sum_{\ell=0}^{L_{j'}-1}\prod_{t_{j'\ell}\in\mathbf{t}^{\mathcal{K}_J\setminus\mathcal{K}_k}} \Pr(T_{ij'}=\ell)\ \ \widehat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_k}, \mathbf{T}_i^{\mathcal{K}_J\setminus\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_J\setminus\mathcal{K}_k}]$$
$$- \sum_{\mathcal{K}_p\subset\mathcal{K}_k}\sum_{\mathbf{t}^{\mathcal{K}_p}} \mathbf{1}\{\mathbf{t}^{\mathcal{K}_p} \subset \mathbf{t}^{\mathcal{K}_k}\}\hat{\beta}^{\mathcal{K}_p}_{\mathbf{t}^{\mathcal{K}_p}} - \hat{\mu}. \tag{24}$$

In addition, $\hat{\mu}$ is given as follows.

$$\hat{\mu} \;=\; \sum_{j=1}^{K}\sum_{\ell=0}^{L_j-1}\prod_{t_{j\ell}\in\mathbf{t}^{\mathcal{K}_J}} \Pr(T_{ij}=\ell)\ \ \widehat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_J} = \mathbf{t}^{\mathcal{K}_J}].$$

Therefore, $(\hat{\mu}, \hat{\boldsymbol{\beta}})$ is uniquely determined. To confirm this solution is the minimizer of the optimization problem, we check all the equality conditions. For all $\mathbf{t}^{\mathcal{K}_k}, \mathcal{K}_k \subset \mathcal{K}_J, j \in \mathcal{K}_k$ and $k \geq 1$,

$$
\begin{aligned}
& \sum_{\ell=0}^{L_j-1} \Pr(T_{ij}=\ell)\mathbf{1}\{t_j=\ell\}\hat{\beta}^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}} \\
= & \sum_{\ell=0}^{L_j-1} \Pr(T_{ij}=\ell)\mathbf{1}\{t_j=\ell\} \sum_{j' \in \mathcal{K}_J \setminus \mathcal{K}_k} \sum_{\ell=0}^{L_{j'}-1} \prod_{t_{j'\ell} \in \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k}} \Pr(T_{ij'}=\ell) \;\; \widehat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_k}, \mathbf{T}_i^{\mathcal{K}_J \setminus \mathcal{K}_k} = \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k}] \\
& \qquad - \sum_{\ell=0}^{L_j-1} \Pr(T_{ij}=\ell)\mathbf{1}\{t_j=\ell\} \sum_{\mathcal{K}_p \subset \mathcal{K}_k} \sum_{\mathbf{t}^{\mathcal{K}_p}} \mathbf{1}\{\mathbf{t}^{\mathcal{K}_p} \subset \mathbf{t}^{\mathcal{K}_k}\} \hat{\beta}^{\mathcal{K}_p}_{\mathbf{t}^{\mathcal{K}_p}} - \hat{\mu} \\
= & \sum_{j' \in \{j, \mathcal{K}_J \setminus \mathcal{K}_k\}} \sum_{\ell=0}^{L_{j'}-1} \prod_{t_{j'\ell} \in \mathbf{t}^{\{j, \mathcal{K}_J \setminus \mathcal{K}_k\}}} \Pr(T_{ij'}=\ell) \;\; \widehat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_k \setminus j} = \mathbf{t}^{\mathcal{K}_k \setminus j}, \mathbf{T}_i^{\{j, \mathcal{K}_J \setminus \mathcal{K}_k\}} = \mathbf{t}^{\{j, \mathcal{K}_J \setminus \mathcal{K}_k\}}] \\
& \qquad - \sum_{\mathcal{K}_p \subseteq \mathcal{K}_k \setminus j} \sum_{\mathbf{t}^{\mathcal{K}_p}} \mathbf{1}\{\mathbf{t}^{\mathcal{K}_p} \subseteq \mathbf{t}^{\mathcal{K}_k \setminus j}\} \hat{\beta}^{\mathcal{K}_p}_{\mathbf{t}^{\mathcal{K}_p}} - \hat{\mu} \\
= & \; 0,
\end{aligned}
$$

where the final equality comes from equation (24) for $\hat{\beta}^{\mathcal{K}_k \setminus j}_{\mathbf{t}^{\mathcal{K}_k \setminus j}}$.

Furthermore, equation (23) implies all other equalities in equation (22). Therefore, the solution (equations (24) and (25)) satisfies all the equality conditions. Finally, we show that these estimators are unbiased for the AMEs and the AMIEs. Since $\widehat{\mathbb{E}}[Y_i \mid \mathbf{T}_i^{\mathcal{K}_J} = \mathbf{t}^{\mathcal{K}_J}]$ is an unbiased estimator of $\mathbb{E}[Y_i(\mathbf{t}^{\mathcal{K}_J})]$,

$$
\begin{aligned}
\mathbb{E}[\hat{\beta}^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}}] &= \sum_{j' \in \mathcal{K}_J \setminus \mathcal{K}_k} \sum_{\ell=0}^{L_{j'}-1} \prod_{t_{j'\ell} \in \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k}} \Pr(T_{ij'}=\ell) \;\; \mathbb{E}[Y_i(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k})] \\
& \qquad - \sum_{\mathcal{K}_p \subset \mathcal{K}_k} \sum_{\mathbf{t}^{\mathcal{K}_p}} \mathbf{1}\{\mathbf{t}^{\mathcal{K}_p} \subset \mathbf{t}^{\mathcal{K}_k}\} \mathbb{E}[\hat{\beta}^{\mathcal{K}_p}_{\mathbf{t}^{\mathcal{K}_p}}] - \hat{\mu}, \\
\mathbb{E}[\hat{\beta}^{\mathcal{K}_k}_{\mathbf{t}^{\mathcal{K}_k}} - \hat{\beta}^{\mathcal{K}_k}_{\mathbf{t}_0^{\mathcal{K}_k}}] &= \sum_{j' \in \mathcal{K}_J \setminus \mathcal{K}_k} \sum_{\ell=0}^{L_{j'}-1} \prod_{t_{j'\ell} \in \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k}} \Pr(T_{ij'}=\ell) \;\; \mathbb{E}[Y_i(\mathbf{t}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k}) - Y_i(\mathbf{t}_0^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_J \setminus \mathcal{K}_k})] \\
& \qquad - \sum_{\mathcal{K}_p \subset \mathcal{K}_k} \sum_{\mathbf{t}^{\mathcal{K}_p}} \mathbf{1}\{\mathbf{t}^{\mathcal{K}_p} \subset \mathbf{t}^{\mathcal{K}_k}\} \mathbb{E}[\hat{\beta}^{\mathcal{K}_p}_{\mathbf{t}^{\mathcal{K}_p}} - \hat{\beta}^{\mathcal{K}_p}_{\mathbf{t}_0^{\mathcal{K}_p}}] \\
&= \pi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k}).
\end{aligned}
$$

□

B Supplementary Appendix: Proofs of Lemmas

For the sake of completeness, we prove all the lemmas used in the mathematical appendix above.

B.1 Proof of Lemma 1

To simplify the proof, we start from Lemma 1 and prove it is equivalent to Definition 3. We prove it by induction. Equation (7) shows this correspondence holds for $K = 2$. Next, choose any $K \geq 2$ and assume that this relationship holds. That is, we assume the following equality,

$$\xi_{\mathcal{K}_K}(\mathbf{t};\mathbf{t}_0) \ = \ \tau_{\mathcal{K}_K}(\mathbf{t};\mathbf{t}_0) \ - \ \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}), \qquad (25)$$

where the second summation is taken over all possible $\mathcal{K}_k \subseteq \mathcal{K}_K = \{1, \ldots, K\}$ with $|\mathcal{K}_k| = k$.

Using the definition of the K-way AIE in Lemma 1, we have,

$$\begin{aligned}
& \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1};\mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
= & \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k} \mid T_{i,K+1} = t_{K+1}, \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
& \quad - \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k} \mid T_{i,K+1} = t_{0,K+1}, \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}), \qquad (26)
\end{aligned}$$

where $\xi_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1};\mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k})$ denote the conditional $(k+1)$-way AIE that includes the set of k treatments, $\mathcal{K}_k$, as well as the $(K+1)$th treatment while fixing $\overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k}$ to $\mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}$. Therefore, we have,

$$\begin{aligned}
& \xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}}) \\
= \ & \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K};\mathbf{t}_0^{\mathcal{K}_K} \mid T_{i,K+1} = t_{K+1}) - \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K};\mathbf{t}_0^{\mathcal{K}_K} \mid T_{i,K+1} = t_{0,K+1}) \\
= \ & \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1};\mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) - \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{0,K+1};\mathbf{t}_0^{\mathcal{K}_K}, t_{0,K+1})
\end{aligned}$$

$$- \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k})$$

$$= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) - \sum_{k=1}^{K} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k})$$

$$- \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}), \tag{27}$$

where the second equality follows from equation (26), and the third equality is based on the application of the assumption given in equation (25) while conditioning on $T_{i,K+1} = t_{0,K+1}$.

Next, consider the following decomposition,

$$\sum_{k=1}^{K} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k})$$

$$= \sum_{k=1}^{K} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k})$$

$$+ \sum_{k=1}^{K-1} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \xi_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k})$$

$$+ \xi_{(K+1)}(t_{K+1}; t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K} = \mathbf{t}_0^{\mathcal{K}_K}), \tag{28}$$

where the first term corresponds to the cases with $K+1 \in \mathcal{K}_{K+1} \setminus \mathcal{K}_k$, while the second and third terms together represent the cases with $K+1 \in \mathcal{K}_k$. Note that these two cases are mutually exclusive and exhaustive. Finally, note the following equality,

$$\tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) \;=\; \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) \;-\; \xi_{(K+1)}(t_{K+1}; t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K} = \mathbf{t}_0^{\mathcal{K}_K}).$$

Then, together with equations (27) and (28), we obtain, the desired result,

$$\xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) \;=\tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) \;-\; \sum_{k=1}^{K} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_{K+1}} \xi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}).$$

Thus, the lemma holds for any $K \geq 2$. □

B.2 Proof of Lemma 2

To begin, we prove the following equality by mathematical induction.

$$\begin{aligned}
&\xi_{\mathcal{K}_K}(\tilde{\mathbf{T}}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_K}) \\
&= \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k}) + \sum_{\ell=1}^{k} (-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}).
\end{aligned} \tag{29}$$

First, it is clear that this equality holds when $k = 1$. That is, for a given $\mathcal{K}_1$, we have,

$$\begin{aligned}
&\xi_{\mathcal{K}_K}(\tilde{T}^{\mathcal{K}_1}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_1}; \mathbf{t}_0^{\mathcal{K}_K}) \\
&= \xi_{\mathcal{K}_K \setminus \mathcal{K}_1}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_1}; \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_1} \mid \tilde{T}_i^{\mathcal{K}_1} = \tilde{t}^{\mathcal{K}_1}) - \xi_{\mathcal{K}_K \setminus \mathcal{K}_1}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_1}; \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_1} \mid T_i^{\mathcal{K}_1} = t_0^{\mathcal{K}_1}).
\end{aligned} \tag{30}$$

Now, assume that the equality holds for k. Without loss of generality, we suppose $\mathcal{K}_k = \{1, 2, \ldots, k\}$ and $\mathcal{K}_{k+1} = \{1, 2, \ldots, k, k+1\}$. By the definition of the K-way AIE,

$$\begin{aligned}
&\xi_{\mathcal{K}_K}(\tilde{\mathbf{T}}^{\mathcal{K}_{k+1}}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}; \mathbf{t}_0^{\mathcal{K}_K}) \\
&= \xi_{\mathcal{K}_K \setminus (k+1)}(\tilde{\mathbf{T}}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}; \mathbf{t}_0^{\mathcal{K}_K \setminus (k+1)} \mid \tilde{T}_i^{k+1}) - \xi_{\mathcal{K}_K \setminus (k+1)}(\tilde{\mathbf{T}}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}; \mathbf{t}_0^{\mathcal{K}_K \setminus (k+1)} \mid T_i^{k+1} = t_0^{k+1}) \\
&= \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}; \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}_i^{\mathcal{K}_{k+1}}) \\
&\quad + \sum_{\ell=1}^{k} (-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_{k+1} \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) \\
&\quad - \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}; \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}_i^{\mathcal{K}_k}, T_i^{k+1} = t_0^{k+1}) \\
&\quad + \sum_{\ell=1}^{k} (-1)^{\ell+1} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}, T_i^{k+1} = t_0^{k+1}),
\end{aligned} \tag{31}$$

where the second equality follows from the assumption.

Next, consider the following decomposition.

$$\sum_{\ell=1}^{k+1} (-1)^\ell \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_{k+1}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_{k+1} \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell})$$

$$
\begin{aligned}
&= \sum_{\ell=1}^{k}(-1)^{\ell} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_{k+1} \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) \\
&\quad - \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}; \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}_i^{\mathcal{K}_k}, T_i^{k+1} = t_0^{k+1}) \\
&\quad + \sum_{\ell=1}^{k}(-1)^{\ell+1} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}, T_i^{k+1} = t_0^{k+1}),
\end{aligned}
\tag{32}
$$

where the first term corresponds to the case in which $\mathcal{K}_\ell \subseteq \mathcal{K}_{k+1}$ in the left side of the equation does not include the $(k+1)$th treatment, and the second and third terms jointly express the case in which $\mathcal{K}_\ell \subseteq \mathcal{K}_{k+1}$ in the left side of the equation does include the $(k+1)$th treatment.

Putting together equations (31) and (32), we have,

$$
\begin{aligned}
&\xi_{\mathcal{K}_K}(\tilde{\mathbf{T}}^{\mathcal{K}_{k+1}}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_K}) \\
&= \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_{k+1}}) \\
&\quad + \sum_{\ell=1}^{k+1}(-1)^{\ell} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_{k+1}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_{k+1}} \mid \tilde{\mathbf{T}}^{\mathcal{K}_{k+1} \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}).
\end{aligned}
$$

Therefore, equation (29) holds in general. Finally, under Assumption 2,

$$
\begin{aligned}
&\int_{\overline{\mathcal{F}}^{\mathcal{K}_k}} \xi_{\mathcal{K}_K}(\tilde{\mathbf{T}}^{\mathcal{K}_k}, \mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_K}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k}) \\
&= \int_{\overline{\mathcal{F}}^{\mathcal{K}_k}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k}) \\
&\quad + \sum_{\ell=1}^{k}(-1)^{\ell} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \int_{\overline{\mathcal{F}}^{\mathcal{K}_k}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k}) \\
&= \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
&+ \sum_{\ell=1}^{k}(-1)^{\ell} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \left\{ \int_{\overline{\mathcal{F}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}} \int_{\overline{\mathcal{F}}^{\mathcal{K}_\ell}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_\ell} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}) \right\} \\
&= \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
&\quad + \sum_{\ell=1}^{k}(-1)^{\ell} \sum_{\mathcal{K}_\ell \subseteq \mathcal{K}_k} \int_{\overline{\mathcal{F}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}} \xi_{\mathcal{K}_K \setminus \mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_K \setminus \mathcal{K}_k}, \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k} \mid \tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}, \overline{\mathbf{T}}_i^{\mathcal{K}_\ell} = \mathbf{t}_0^{\mathcal{K}_\ell}) dF(\tilde{\mathbf{T}}^{\mathcal{K}_k \setminus \mathcal{K}_\ell}).
\end{aligned}
$$

This completes the proof of Lemma 2. □

B.3 Proof of Lemma 3

We prove the lemma by induction. For $K = 2$, equation (7) shows that the lemma holds. Choose any $K \geq 2$ and assume that the lemma holds for all k with $1 \leq k \leq K$. Then,

$$\begin{aligned}
&\xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K} \mid T_{i,K+1} = t_{K+1}) \\
&= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) + \sum_{k=1}^{K-1} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, t_{K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
&= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) \\
&\quad + \sum_{k=1}^{K-1} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \Big[\tau_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
&\qquad\qquad - \tau_{K+1}(t_{K+1}; t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \ (K+1)} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \ (K+1)}) \Big] \\
&= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) \\
&\quad + \sum_{k=1}^{K-1} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\{\mathcal{K}_k, K+1\}}(\mathbf{t}^{\mathcal{K}_k}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_k}, t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_K \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_K \setminus \mathcal{K}_k}) \\
&\quad + \sum_{k=1}^{K-1} (-1)^{K-k+1} \binom{K}{k} \tau_{K+1}(t_{K+1}; t_{0,K+1} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \ (K+1)} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \ (K+1)}). \qquad (33)
\end{aligned}$$

Next, note the following decomposition,

$$\begin{aligned}
\xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) &= \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K} \mid T_{i,K+1} = t_{K+1}) - \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_L} \mid T_{i,K+1} = t_{0,K+1}) \\
&= \xi_{\mathcal{K}_K}(\mathbf{t}^{\mathcal{K}_K}; \mathbf{t}_0^{\mathcal{K}_K} \mid T_{i,K+1} = t_{K+1}) \\
&\quad - \sum_{k=1}^{K} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k}).
\end{aligned}$$

Substituting equation (33) into this equation, we obtain

$$\begin{aligned}
&\xi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}}; \mathbf{t}_0^{\mathcal{K}_{K+1}}) \\
&= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K}, t_{K+1}; \mathbf{t}_0^{\mathcal{K}_K}, t_{K+1}) - \sum_{k=1}^{K} (-1)^{K-k} \sum_{\mathcal{K}_k \subseteq \mathcal{K}_K} \tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k}; \mathbf{t}_0^{\mathcal{K}_k} \mid \overline{\mathbf{T}}_i^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k} = \mathbf{t}_0^{\mathcal{K}_{K+1} \setminus \mathcal{K}_k})
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{k=1}^{K-1}(-1)^{K-k}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_K}\tau_{\{\mathcal{K}_k,K+1\}}(\mathbf{t}^{\mathcal{K}_k},t_{K+1};\mathbf{t}_0^{\mathcal{K}_k},t_{0,K+1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_K\setminus\mathcal{K}_k}=\mathbf{t}_0^{\mathcal{K}_K\setminus\mathcal{K}_k})\\
&+\sum_{k=1}^{K-1}(-1)^{K-k+1}\binom{K}{k}\tau_{K+1}(t_{K+1};t_{0,K+1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\ (K+1)}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\ (K+1)})\\
=\ &\tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_K},t_{K+1};\mathbf{t}_0^{\mathcal{K}_K},t_{K+1})-\sum_{k=2}^{K}(-1)^{K-k}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}}\tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k})\\
&+(-1)^K\sum_{\mathcal{K}_1\subseteq\mathcal{K}_K}\tau_{\mathcal{K}_1}(t^{\mathcal{K}_1},t_0^{\mathcal{K}_1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\ \mathcal{K}_1}=\mathbf{t}_0^{\mathcal{K}_{L+1}\setminus\ \mathcal{K}_1})\\
&+\sum_{k=1}^{K-1}(-1)^{K-k+1}\binom{K}{k}\tau_{K+1}(t_{K+1};t_{0,K+1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\ (K+1)}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\ (K+1)})\\
=\ &\tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}})-\tau_{K+1}(t_{K+1};t_{0,K+1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\ (K+1)}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\ (K+1)})\\
&-\sum_{k=2}^{K}(-1)^{K-k}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}}\tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}=\mathbf{t}_0^{\mathcal{K}_{K+k}\setminus\mathcal{K}_k})\\
&+(-1)^K\sum_{\mathcal{K}_1\subseteq\mathcal{K}_K}\tau_{\mathcal{K}_1}(t^{\mathcal{K}_1},t_0^{\mathcal{K}_1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\ \mathcal{K}_1}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\ \mathcal{K}_1})\\
&+\sum_{k=1}^{K-1}(-1)^{K-k+1}\binom{K}{k}\tau_{K+1}(t_{K+1};t_{0,K+1}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\ (K+1)}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\ (K+1)})\\
=\ &\sum_{k=1}^{K+1}(-1)^{K-k+1}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}}\tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k}\mid\overline{\mathbf{T}}_i^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}=\mathbf{t}_0^{\mathcal{K}_{K+1}\setminus\mathcal{K}_k}),
\end{aligned}
$$

where the final equality follows because

$$
-1+\sum_{k=1}^{K-1}(-1)^{K-k+1}\binom{K}{k}\ =\ (-1)^K.
$$

Thus, by induction, the theorem holds for any $K \geq 2$. □

B.4 Proof of Lemma 4

We prove the lemma by induction. For $K = 2$, equation (7) shows this theorem holds. Choose any $K \geq 2$ and assume that the lemma holds for all k with $1 \leq k \leq K$. That is, let $\mathcal{K}_k \subseteq \mathcal{K}_K = \{1, \ldots, K\}$ with $|\mathcal{K}_k| = k$ where $k = 1, \ldots, K$, and assume the following equality,

$$
\pi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k})\ =\ \sum_{\ell=1}^{k}(-1)^{k-\ell}\sum_{\mathcal{K}_\ell\subseteq\mathcal{K}_k}\tau_{\mathcal{K}_\ell}(\mathbf{t}^{\mathcal{K}_\ell};\mathbf{t}_0^{\mathcal{K}_\ell}).
$$

Using this assumption as well as the definition of the K-way AMIE given in Definition 2, we have,

$$\begin{aligned}\pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}}) &= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}}) - \sum_{k=1}^{K}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}} \pi_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k}) \\ &= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}}) + \sum_{k=1}^{K}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}}\sum_{\ell=1}^{k}(-1)^{k+1-\ell}\sum_{\mathcal{K}_\ell\subseteq\mathcal{K}_k}\tau_{\mathcal{K}_\ell}(\mathbf{t}^{\mathcal{K}_\ell};\mathbf{t}_0^{\mathcal{K}_\ell}).\end{aligned} \tag{34}$$

Next, we determine the coefficient for $\tau_{\mathcal{K}_m}(\mathbf{t}^{\mathcal{K}_m};\mathbf{t}_0^{\mathcal{K}_m})$ in the second term of equation (34) for each m with $1 \leq m \leq K$. Note that $\tau_{\mathcal{K}_m}(\mathbf{t}^{\mathcal{K}_m};\mathbf{t}_0^{\mathcal{K}_m})$ would not appear in this term if $m > k$. That is, for a given m, we only need to consider the cases where the index for the first summation satisfies $m \leq k \leq K$. Furthermore, for any given such k, there exist $\binom{K+1-m}{k-m}$ ways to choose $\mathcal{K}_k$ in the second summation such that $\mathcal{K}_m \subseteq \mathcal{K}_k$. Once such $\mathcal{K}_k$ is selected, $\mathcal{K}_m$ appears only once in the third and fourth summations together and is multiplied by $(-1)^{k+1-m}$. Therefore, the coefficient for $\tau_{\mathcal{K}_m}(\mathbf{t}^{\mathcal{K}_m};\mathbf{t}_0^{\mathcal{K}_m})$ is equal to,

$$\sum_{k=m}^{K}(-1)^{k+1-m}\binom{K+1-m}{k-m} = (-1)^{K+1-m}.$$

Putting all of these together,

$$\begin{aligned}\pi_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}}) &= \tau_{\mathcal{K}_{K+1}}(\mathbf{t}^{\mathcal{K}_{K+1}};\mathbf{t}_0^{\mathcal{K}_{K+1}}) + \sum_{k=1}^{K}(-1)^{K+1-k}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}}\tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k}) \\ &= \sum_{k=1}^{K+1}(-1)^{K+1-k}\sum_{\mathcal{K}_k\subseteq\mathcal{K}_{K+1}}\tau_{\mathcal{K}_k}(\mathbf{t}^{\mathcal{K}_k};\mathbf{t}_0^{\mathcal{K}_k}).\end{aligned}$$

Since the theorem holds for $K + 1$, we have shown that it holds for any $K \geq 2$. □