A Markovian Approach for Cross-Category Complementarity in Choice Modeling

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Abstract. While single-purchase choice models have been widely studied in assortment optimization, customers in modern retail and e-commerce environments often purchase multiple items across distinct product categories, exhibiting both substitution and complementarity. We consider the cross-category assortment optimization problem where retailers jointly determine assortments across categories to maximize expected revenue. Most prior work on the topic either overlooks complementarity or proposes models that lead to intractable optimization problems, despite being based on the multinomial logit (MNL) choice model. We propose a sequential multi-purchase choice model for cross-category choice that incorporates complementarity through a Markovian transition structure across categories, while allowing general Random Utility Maximization (RUM)-based choice models to capture the within-category substitution. We develop an Expectation-Maximization algorithm for estimation, and a polynomial-time algorithm for unconstrained assortment optimization that yields the optimal solution when the within-category substitution follows a Markov chain choice model.

Furthermore, we introduce an empirical metric to quantify complementarity strength across product categories and conduct extensive numerical experiments on both synthetic data and a large-scale transaction-level dataset from a major US grocery store. Our model yields improvements in predictive accuracy, model fit, and expected revenue in setting with complementarity, and it reveals intuitive market structures such as brand-loyal cross-category purchasing. Overall, we believe that our model provides a theoretically-grounded and practical framework for modeling complementarity and making better cross-category assortment decisions.

1. Introduction

Customers frequently make purchases that span multiple product categories within a single transaction. In retail settings, for instance, a shopper might select products from several different categories. A large-scale study of U.S. and U.K. supermarkets found that 83% of transactions involved products from more than one category (Tanusondjaja et al. 2016). This phenomenon extends beyond retail to service industries such as airlines, where a traveler first books a flight and then makes sequential choices on ancillary services. When purchases span multiple categories, a choice in one category often alters a customer's preferences in another. The marketing and economics literature provides strong empirical support for these cross-category dependencies, also known as *complementarity* effects (Mulhern and Leone 1991, Aurier and Mejía 2014, Kwak et al. 2015).

In many settings, customers' choices unfold in a sequential manner across related product categories. Typically, shoppers begin by selecting a focal or primary product (e.g., a cell phone, TV, cake mix, or flight), which subsequently shapes their decisions regarding complementary products (e.g., a phone case, TV bracket, cake frosting, or add-on services). This directional dependency is often referred to in the marketing literature as asymmetric complementarity (Manchanda et al. 1999, Lee et al. 2013). For instance, the price of cake mix has been shown to substantially influence frosting sales, whereas the reverse effect is considerably weaker (Mulhern and Leone 1991, Manchanda et al. 1999). Similar one-way relationships have been documented between spaghetti and spaghetti sauce (Walters 1991), as well as between laundry detergent and fabric softener (Manchanda et al. 1999). This asymmetric complementarity is also prominent in digital ecosystems, where the purchase of an e-reader drives subsequent e-book sales (Li 2019). Such asymmetric patterns may emerge for several reasons, including the logic of product usage, in-store merchandising strategies, or consumers' cognitive decision-making processes. Moreover, in many settings, customers have higher willingness to pay for primary products than for complementary products, so the influence of primary products tends to dominate the reverse effect (Ke and Wang 2022).

Optimizing assortments across interdependent categories poses a significant managerial challenge in many industries. In grocery retail, for instance, jointly managing assortments of primary products such as cake mixes alongside their complements like frosting can increase both sales and profitability. In e-commerce, coordinating assortments of core products with compatible accessories at the fulfillment-center level can enhance customer experience and stimulate cross-selling, for example, offering phones together with chargers or protective cases increases the likelihood of bundled purchases. Similarly, auto dealerships must decide not only which vehicle models and trims to stock but also how to design a profitable portfolio of accessories and extended service plans. In the travel industry, assortment decisions on airline routes and fare classes are closely linked to the design of ancillary offerings such as seat upgrades and partner hotel bookings, which often significantly boost profitability.

Despite its practical importance and a long tradition of studying complementarity in economics and marketing, this phenomenon remains underexplored in the assortment optimization literature. Most existing work has focused primarily on modeling substitution effects within a single category, typically using variants of the multinomial logit (MNL), nested logit, or Markov chain (MC) models. However, ignoring cross-category dependencies can lead to suboptimal assortments and significant profit losses (Ghoniem et al. 2016). To date, no standard framework exists for modeling and optimizing assortments in general cross-category settings. Models that do incorporate complementarity often rely on heuristics without theoretical guarantees or become computationally intractable as the number of products and categories increases (Ghoniem et al. 2016, Ke and Wang 2022, Chen et al. 2022, Tulabandhula et al. 2023). Moreover, while most prior studies employ the MNL to capture substitution within each category, the broader discrete choice literature offers richer generalizations that may be more suitable for practice. Finally, most prior work has emphasized algorithm design under a given model, while giving less attention to model realism and ease of estimation.

In this paper, we address these gaps by proposing a practical yet theoretically grounded model that captures cross-category complementarity, remains tractable for large-scale assortment optimization, and supports efficient estimation.

1.1. Summary of Our Results

Our contributions are threefold. First, we introduce a general and estimable multi-purchase choice model that captures cross-category complementarity while remaining tractable for large-scale assortment optimization. Second, we establish the tractability of the multi-category assortment optimization problem when substitution within each category is captured by Markov chain choice models, showing that joint optimization is possible across multiple categories. Third, we empirically validate the model using both synthetic and large-scale retail data, demonstrating improved predictive performance, significant revenue gains, and actionable managerial insights into the strength and heterogeneity of cross-category complementarity.

Model. At the core of our work is a novel Markovian multi-purchase choice model in which customers sequentially navigate multiple product categories. To build intuition, we first discuss the model for two categories: a primary and a secondary. Within each category, choices are governed by a general random-utility-based model (e.g., a MC model or a simpler MNL model). After selecting a product in the primary category, the customer transitions to the secondary category in a Markovian manner. More specifically, they transition to their most favorable product in the secondary category with a certain probability. This transition probability depends on the choice in the first category, thereby capturing complementarity between the primary and secondary products. If the most preferred product is included in the offered assortment, the customer purchases it and exits; otherwise, they substitute among the available options using the within-category choice model, conditional on the originally preferred product.

This approach contrasts with prior work, which typically extends single-purchase MNL models by assuming that a primary choice redefines the entire set of preference weights in the secondary category. Instead, we retain a fixed within-category choice model for the secondary category, with the primary choice determining only the first preferred product rather than reshaping the full preference structure. Our framework naturally extends to more general settings where categories follow a directed acyclic graph (DAG) structure (see Section 2.2).

Assortment optimization. A key advantage of our approach is that it enables tractable, unconstrained assortment optimization under the MC choice model, even with an arbitrary number of categories. At first glance, the problem seems daunting: assortments must be chosen jointly across categories, and these decisions are inherently interdependent. Tractability arises, however, because with appropriate adjustments to product prices the optimization problem naturally decouples. In particular, the choice in one category affects only the initial arrival probabilities in the next category's MC model, and there exists an optimal assortment for an MC model that is invariant to these initial probabilities. Consequently, the overall problem can be solved sequentially, category by category, following an appropriate ordering of categories.

This scalability represents a substantial improvement over existing multi-purchase choice models, which are often restricted to two categories. In contrast, our model accommodates an arbitrary number of categories without sacrificing tractability. Note that single-category assortment optimization does not admit a polynomial-time constant-factor approximation algorithm under a general Random Utility Maximization (RUM)-based choice model (Aouad et al. 2018). For this reason, we focus on the MC model, which is both expressive and tractable for single-category assortment optimization. Other within-category models with known tractability, such as the nested logit model, could also be considered; however, the tractability of joint optimization under such non-Markovian choice models (Li and Udwani 2023) remains an open and challenging direction for future research.

Empirical validation and managerial insights. The central question for assessing our model's practical value is whether it can effectively capture complementarity in transaction data. After all, tractable optimization and estimation could be achieved by simply treating each category independently, but this would ignore cross-category dependencies that may be crucial in practice. To address this, we develop an efficient Expectation–Maximization (EM) algorithm for estimation and validate our model through extensive experiments using both real and synthetic data.

Our real-world empirical analysis is based on a dataset of over 6.2 million transactions from a major U.S. grocery retailer. We first introduce a new metric to quantify cross-category complementarity and apply it to identify product categories that exhibit strong and heterogeneous dependencies. For these categories, our model significantly outperforms benchmarks that ignore cross-category effects, achieving superior fit and prediction accuracy, while performing on par with existing state-of-the-art models for asymmetric complementarity. In addition, parameter estimates reveal complementary relationships at the product level, for example, customers who purchase a specific brand of cake mix exhibit a markedly stronger preference for the corresponding brand of frosting. These findings highlight how our framework can generate actionable insights for operational strategies beyond assortment optimization, such as coordinated pricing, promotions, and store layout design.

We also construct a synthetic dataset that allows us to systematically vary the strength of complementarity and test the performance of our assortment optimization algorithm. Results show that our model consistently outperforms benchmarks in both predictive performance and expected revenue. Importantly, the revenue gains increase with the strength of complementarity: in settings with strong cross-category dependence, our model delivers 6–10% higher expected revenue relative to a benchmark that ignores complementarity.

Outline. The remainder of this paper is organized as follows. In Section 1.2, we review the relevant literature. In Section 2, we introduce our sequential multi-purchase choice model. In Section 3, we introduce the corresponding assortment optimization problem, provide a polynomial-time algorithm for the unconstrained case, and establish the hardness of the cardinality-constrained problem. In Section 4, we develop an Expectation-Maximization algorithm for model estimation. Section 5 validates the model on synthetic data, and Section 6 applies it to a large-scale retail dataset to demonstrate practical value. Section 7 concludes with a summary of findings and directions for future research.

1.2. Related Work

The literature on single-purchase assortment optimization is extensive. Efficient algorithms have been developed under various choice models, such as MNL (Talluri and Van Ryzin 2004, Gallego et al. 2004, Rusmevichientong et al. 2010), mixed MNL (Bront et al. 2009), nested logit (Davis et al. 2014), and Markov chain choice models (Blanchet et al. 2016, Feldman and Topaloglu 2017, Désir et al. 2020). For comprehensive surveys, we refer the reader to Kök et al. (2015), Strauss et al. (2018), and Heger and Klein (2024). In this section, we focus on reviewing related work on complementarity modeling and assortment optimization with complementarity. We also review multi-purchase choice models that focus on substitution effects only.

Complementarity in marketing and economics. Modeling product complementarity has a long history in marketing and economics, where the literature focuses on estimation and interpretation of model parameters rather than optimization. This stream of work typically classifies complementarity as either *symmetric* or *asymmetric*, depending on whether purchase order influences the complementarity effect (Seetharaman et al. (2005), Lee et al. (2013), Aurier and Mejía (2014), Kwak et al. (2015)). For instance, Lee et al. (2013) propose a direct utility model with a latent decision sequence across categories to measure the asymmetric complementarity effects. Ruiz et al. (2019) develop a sequential probabilistic model of customers' shopping baskets, where customers select products sequentially and each choice is conditional on products already in the basket. Recent work in recommender systems applies machine learning methods to identify substitutable and complementary products (McAuley et al. 2015, Tkachuk et al. 2022). However, these models are primarily designed for prediction and estimation, and do not readily extend to assortment optimization.

Assortment optimization with product complementarity. Our work is most closely related to recent research on assortment optimization under asymmetric complementarity, which typically assumes a sequential purchase structure where an initial choice influences subsequent ones. The closest paper is Ke and Wang (2022), which models a two-stage process: customers first select a primary product using an MNL model, then make a secondary choice from another category using an MNL model whose parameters depend on the first selection. The authors consider two settings: a personalized one, where the secondary assortment can be tailored to the initial purchase, and a non-personalized one, where the same secondary assortment is offered to all customers. The personalized setting is straightforward to solve in both Ke and Wang (2022) and our framework (see Section 3.1 for details). We focus instead on the non-personalized setting, which is more relevant for brick-and-mortar retailers that cannot adjust assortments in real time, and is also more technically challenging. In this setting, Ke and Wang (2022) show that the unconstrained assortment problem is NP-hard even for two categories. In contrast, our model admits a tractable algorithm for the unconstrained case, accommodates more general within-category choice models (e.g., MC model), and extends to an arbitrary number of categories. While Ke and Wang (2022) also study pricing, we defer this dimension to future work. Other works have explored the joint assortment and pricing problem for complementary categories, proposing mixed-integer programming formulations (Ghoniem et al. 2016) or stylized models (Rodríguez and Aydın 2011). Another line of research models asymmetric complementarity but considers a single-purchase setting. For example, Lo and Topaloglu (2019) examine how the presence of one product can asymmetrically influence the utility of another. This differs from our framework, where complementarity arises from actual purchases and occurs across categories. A related stream considers personalized recommendations conditioned on a given primary choice (Chen et al. 2024, Ban et al. 2024). A key distinction is that in our model, the primary product is not exogenously given but is part of the endogenous customer choice process. Moreover, we focus on determining a single/static assortment offered to all customers, rather than an assortment that adapts dynamically to their prior selections.

For symmetric complementarity, recent research considers assortment optimization under variants of multivariate (MVMNL) models. In these models, substitution and complementarity are captured through a 'bundle' utility that combines individual product utilities with pairwise interaction terms (Chen et al. 2022, Jasin et al. 2024, Tulabandhula et al. 2023). Chen et al. (2022) study a two-category problem and propose a 0.74-approximation algorithm for the unconstrained case, but show that the capacitated version admits no constant-factor approximation (under the Exponential Time Hypothesis). Jasin et al. (2024) develop a Fully Polynomial Time Approximation Scheme (FPTAS) for a variant with group-based interactions for both uncapacitated and capacitated assortment problems, allowing an arbitrary number of groups. Tulabandhula et al. (2023) examine another MVMNL variant where customers can buy at most K products and show the unconstrained problem is NP-hard even when $K = 2$.

Currently, all models incorporating complementarity rely on MNL-based structures. In contrast, our model accommodates more general within-category choice models, such as the MC model. Moreover, whereas prior work establishes NP-hardness even in the unconstrained case, we show that our framework admits tractable unconstrained optimization when within-category choices follow an MC model.

Multi-purchase assortment with substitution effects only. Finally, we review multi-purchase models that consider only substitution effects. Benson et al. (2018) introduce an MNL-based multi-purchase choice model where the total number of products purchased is determined first, after which the specific selections are made. Gallego et al. (2019) propose a choice model termed the Threshold Utility Model (TUM), where a product is purchased if its utility meets or exceeds a threshold, subject to a constraint on the maximum bundle size. While TUM captures realistic multiple-purchase behavior and has favorable analytical properties, the authors do not address the corresponding assortment optimization problem. Immorlica et al. (2021) consider assortment optimization where a value function over bundles encodes substitutability. In their framework, customers choose the subset of products that maximizes this value minus the total price. More recently, Bai et al. (2024) propose a multi-purchase MNL model where customers sample random utilities and purchase the M highest utility products, with M drawn from a known distribution, and propose two Polynomial Time Approximation Schemes (PTAS) for the assortment problem.

2. Model

In this section, we formally introduce our multi-category choice model. We begin by defining the model for two categories and then extend it to more general, multi-category structures.

2.1. Choice Model with Two Categories

At a high level, our model uses a general ranking-based choice model (RCM) to capture substitution effects within each category, and model the complementarity effect between categories through a Markovian transition structure. We first recall the RCM and then introduce our model for two categories.

In RCM, customer preferences are represented by a probability distribution $\mathbf{p}$ over a set $\mathbf{\Sigma}$ of all rankings over the universal set $\mathbf{N}^+ = \mathbf{N} \cup \{0\}$. Each ranking $\sigma \in \mathbf{\Sigma}$ is a permutation of $\mathbf{N}^+$, where a lower value corresponds to a higher preference. That is, $\sigma(i) < \sigma(j)$ implies product i is preferred over product j. Given an offered assortment $S \subseteq \mathbf{N}$, a customer draws a ranking σ according to $(p_\sigma)_{\sigma \in \mathbf{\Sigma}}$ and selects the most preferred product. The choice probability of product $i \in S$ is:

$$\phi(i, S) = \sum_{\sigma \in \mathbf{\Sigma}} \mathbb{1}\left\{ i = \arg \min_{j \in S \cup \{0\}} \sigma(j) \right\} p_\sigma.$$

It is known that RCM is equivalent to RUM-based choice models.

Let A and B denote two product categories, with ground sets $\mathbf{N}_A = \{1, \ldots, n_A\}$ and $\mathbf{N}_B = \{1, \ldots, n_B\}$, respectively. Each category contains a no-purchase option, denoted 0_A for A and 0_B for B. We refer to the full set of options as $\mathbf{N}_A^+ = \mathbf{N}_A \cup \{0_A\}$ and $\mathbf{N}_B^+ = \mathbf{N}_B \cup \{0_B\}$. For assortments $S_A \subseteq \mathbf{N}_A$ and $S_B \subseteq \mathbf{N}_B$, we define the extended assortments $S_A^+ = S_A \cup \{0_A\}$ and $S_B^+ = S_B \cup \{0_B\}$. We use ϕ_A and ϕ_B to denote the RCM models for A and B, respectively.

Now, we introduce our two-category model, which is visualized in Figure 1. The choice process proceeds as follows: the customer first selects $i \in S_A^+$ according to ϕ_A. Unlike prior work that uses this choice to induce a new set of parameters for category B, our model uses i to determine an *initial attraction* toward some $j \in \mathbf{N}_B^+$. This initial attraction is governed by a vector of transition probabilities $\boldsymbol{\lambda}^i = (\lambda_{i,j})_{j \in \mathbf{N}_B^+}$, which satisfies $\sum_{j \in \mathbf{N}_B^+} \lambda_{i,j} = 1$. The dependence of $\boldsymbol{\lambda}^i$ on i is the key feature that captures heterogeneous complementarity. Once the initial attraction is determined, the choice i from category A has no further influence. This is the Markovian property of the model: the subsequent choice behavior in category B depends only on the initial attracted product and is conditionally independent of i. If the attracted product ℓ is available ($\ell \in S_B^+$), the customer purchases it and exits. If $\ell \notin S_B^+$, the customer substitutes among the products in S_B^+ according to ϕ_B, conditioned on ℓ being the top-ranked product in $\mathbf{N}_B^+$.

Formally, let $\mathbf{\Sigma}_\ell = \left\{\sigma \in \mathbf{\Sigma} : \ell = \arg\min_{k\in\mathbf{N}_B^+} \sigma(k)\right\}$ denote the set of all rankings where ℓ is the top-ranked product in $\mathbf{N}_B^+$. The conditional probability that a customer has rank order $\sigma \in \mathbf{\Sigma}_\ell$ is given by $p(\sigma \mid \mathbf{\Sigma}_\ell) = \frac{p_\sigma}{\sum_{\delta\in\mathbf{\Sigma}_\ell} p_\delta}$. The probability that customer selects $j \in S_B^+$, given an initial attraction to a product $\ell \notin S_B^+$, is given by

$$\phi_B(j, S_B \mid \ell) = \sum_{\sigma\in\mathbf{\Sigma}_\ell} p(\sigma \mid \mathbf{\Sigma}_\ell)\, \mathbb{1}\left\{ j = \arg\min_{k\in S_B^+} \sigma(k) \right\}.$$

If $\mathbf{\Sigma}_\ell = \emptyset$, we define $\phi_B(j, S_B \mid \ell) = 0$ for all $j \in S_B^+$. Combining the direct purchase and substitution cases, the overall probability of choosing $i \in S_A^+$ and then $j \in S_B^+$ is

$$P(i, j, S_A, S_B) = \phi_A(i, S_A) \left(\lambda_{i,j} + \sum_{\ell\in\mathbf{N}_B\setminus S_B} \lambda_{i,\ell}\, \phi_B(j, S_B \mid \ell) \right). \tag{1}$$

The first term corresponds to being directly attracted to j, while the second term accounts for attraction to an unavailable product ℓ, followed by substitution to j.

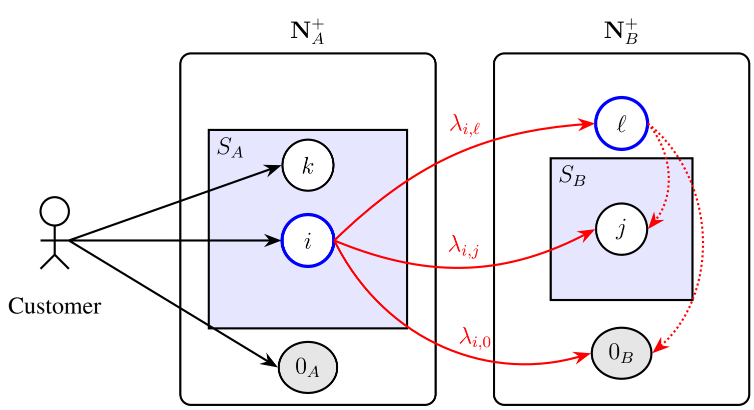


Figure 1 **Diagram of the choice model with two categories.**

Observe that if $\boldsymbol{\lambda}^i$ is the same for all i, then cross-category complementarity vanishes, and the two-category model reduces to two independent choice models. Note that ranking-based choice models include the MNL and MC models as special cases. While our framework allows for general

RCMs to capture substitution, even the single-category unconstrained assortment problem under a general RCM is NP-hard to approximate (Aouad et al. 2018). Therefore, we focus on settings where the within-category choice models ϕ_A and ϕ_B are either MNL or MC, for which single-category assortment optimization is tractable. Our choice of these two particular models is further motivated by two factors. First, using the MNL model enables direct comparison with the existing literature, which is predominantly MNL-based. Second, as we will show, the structure of the MC model is critical for achieving tractable assortment optimization within our framework.

2.1.1. Special Case: Multinomial Logit (MNL) We first analyze the special case where both ϕ_A and ϕ_B are MNL models, to establish a clear connection with the existing literature. In the MNL formulation, the probability of choosing product k from an assortment S is $\phi(k,S) = \frac{v_k}{\sum_{i\in S} v_i + v_0}$, where v_k is the preference weight of product k and v_0 is the weight of the no-purchase option (typically normalized to 1). We use superscripts A and B to denote the weights for categories A and B, respectively.

In this case, the customer first selects product i from S_A^+ with probability $\frac{v_i^A}{\sum_{k\in S_A} v_k^A + 1}$, following the standard MNL model. We then consider the conditional choice probability for product j in S_B^+, given that i was chosen in category A. With probability $\lambda_{i,j}$, the customer is directly attracted to j and purchases it. Alternatively, with probability $\lambda_{i,k}$, the customer is initially attracted to a product $k \notin S_B$ and then substitutes according to $\phi_B(\cdot|k)$. In case of the MNL model, the Independence of Irrelevant Alternatives (IIA) property implies that this distribution is independent of k:

$$\phi_B(j, S_B|k) = \phi_B(j, S_B) \quad \text{for any } k \in \mathbf{N}_B \setminus S_B \text{ and } j \in S_B^+. \tag{2}$$

We show this formally in Lemma 3 in Appendix A.1. Thus, the customer substitutes according to the same MNL distribution ϕ_B. Combining (1) and (2), we obtain the following lemma.

LEMMA 1. *In the MNL special case, given assortments $S_A \subseteq \mathbf{N}_A$ and $S_B \subseteq \mathbf{N}_B$, the joint probability of selecting $i \in S_A^+$ in category A and then $j \in S_B^+$ in category B is*

$$P(i,j,S_A,S_B) = \frac{v_i^A}{V^A(S_A)+1}\left(\lambda_{i,j} + \frac{v_j^B}{V^B(S_B)+1}\sum_{m\in \mathbf{N}_B\setminus S_B} \lambda_{i,m}\right),$$

where $V^A(S_A) = \sum_{k\in S_A} v_k^A$ and $V^B(S_B) = \sum_{k\in S_B} v_k^B$.

Comparison to other MNL-based models. When there is no complementarity (i.e., $\boldsymbol{\lambda}^i$ is the same for all $i \in \mathbf{N}_A^+$), our model reduces to two independent MNL models. We now compare our formulation to other related two-category models. In the model of Ke and Wang (2022), customers first select from S_A^+ according to an MNL model with parameters $(w_i^A)_{i\in\mathbf{N}_A}$. Conditioning on choice i, the customer then selects from B according to another MNL with weights $(w_{i,j})_{j\in\mathbf{N}_B}$, which depend on i. By contrast, our model does not assume a separate conditional MNL; instead, the first-stage choice affects only the initial attraction probabilities in B. The multivariate MNL model of Chen et al. (2022) captures symmetric complementarity by assigning a preference weight u_{ij} to each bundle $(i,j)\in\mathbf{N}_A^+\times\mathbf{N}_B^+$, with the choice probability of a bundle proportional to its weight. Our special case is structurally distinct from both models. In Appendix A.2, we formally show that neither their models nor our MNL-based special case reduce to one another.

Cao et al. (2023) propose a single-purchase model in which the choice probability is a convex combination of an MNL component and an independent demand component. In our model, for any given assortment S_A, the induced choice model in category B has the following choice probabilities for any product $j\in S_B$: $\sum_{i\in S_A^+}\frac{v_i^A}{V^A(S_A)+1}\left(\lambda_{i,j}+\frac{v_j^B}{V^B(S_B)+1}\sum_{m\in\mathbf{N}_B\setminus S_B}\lambda_{i,m}\right)$. At first glance, this form appears similar to the mixture model of Cao et al. (2023) in that both contain an MNL term and an independent demand term. However, the models differ fundamentally: in Cao et al. (2023), the mixture proportion is a fixed parameter, whereas in our model it is endogenously determined by both the offered assortment S_B and the specific first-category choice $i\in S_A$. A detailed comparison is provided in Appendix A.3.

2.1.2. Special Case: Markov Chain (MC) We first recall the definition of an MC model. A standard Markov chain choice model is defined by an initial arrival probability vector $\boldsymbol{\psi}=(\psi_i)_{i\in\mathbf{N}}$ and a transition matrix $\boldsymbol{\rho}=(\boldsymbol{\rho}_{i,k})_{i,k\in\mathbf{N}^+}$ (Blanchet et al. 2016). The choice process begins with an initial attraction to product $i\in\mathbf{N}^+$ with probability ψ_i. If $i\in S^+$, or if it is the no-purchase option, the process terminates and i is chosen. Otherwise, if $i\notin S^+$, the customer transitions to a new product $k\in\mathbf{N}^+$ with probability $\boldsymbol{\rho}_{i,k}$, and this process repeats until an available product or the outside option is reached. For our two-category setting, ϕ_A and ϕ_B are parameterized by $(\boldsymbol{\psi}^A,\boldsymbol{\rho}^A)$ and $(\boldsymbol{\psi}^B,\boldsymbol{\rho}^B)$, respectively.

In our two-category model, after a customer selects i from S_A^+, they form an initial attraction to an item j from category B. If $j\notin S_B^+$, then the customer transitions from j to $\ell\in\mathbf{N}_B^+$ with probability $\boldsymbol{\rho}_{j,\ell}^B$. Overall, the substitution process is equivalent to a MC model that retains the transition matrix $\boldsymbol{\rho}^B$ but sets the initial arrival to product j. Thus, conditioned on i being chosen from A, the choice process in category B is an MC model with initial arrival distribution $\boldsymbol{\lambda}^i$ and transition matrix $\boldsymbol{\rho}^B$.

LEMMA 2. *When the within-category model ϕ_B is a Markov chain choice model with parameters $(\boldsymbol{\psi}^B, \boldsymbol{\rho}^B)$, conditioning on i being chosen from category A, the induced choice process in category B is equivalent to a Markov chain choice model with parameters $(\boldsymbol{\lambda}^i, \boldsymbol{\rho}^B)$.*

Our model for category B differs from a standard MC model in a critical way: instead of relying on a single fixed initial distribution $\boldsymbol{\psi}^B$, it uses $\boldsymbol{\lambda}^i$ that depends on the first-stage choice i from category A. This dependency allows the initial choice to directly shape preferences in category B, thereby capturing complementarity. The substitution dynamics within B, governed by $\boldsymbol{\rho}^B$, remain the same as in the standard MC model. If all $\boldsymbol{\lambda}^i$ were identical across $i \in \mathbf{N}_A^+$, the complementarity would disappear, and the model in category B would reduce to a standard MC choice model.

2.2. Beyond Two Categories

A key feature of our model is its extensibility to settings with more than two categories. We represent cross-category dependencies using a directed acyclic graph (DAG) $G = (\mathcal{V}, \mathcal{E})$. Each vertex $U \in \mathcal{V}$ corresponds to a product category, and each directed edge $(U, W) \in \mathcal{E}$ represents a potential transition from U to W after a choice in U; in this relationship, we refer to U as the parent and W as the child. While DAGs have previously been used to model preferences over individual products in single-purchase settings (Lo and Topaloglu 2019, Jagabathula et al. 2022), we use them here to capture dependencies among categories.

The customer journey through the categories follows a sequence consistent with the graph structure. The process begins with the categories with no dependencies (root nodes). A customer considers a category W only after they have made a choice in all of its parent categories. For a category U with multiple subsequent categories, the customer proceeds to consider each child category in parallel.

This framework can accommodate several common purchasing patterns, as illustrated in Figure 2. A chain structure (left) represents a sequential process, as in project-based shopping like building a PC, where each category's choice depends on the product chosen in its predecessor. A convergent structure (middle) models multiple independent categories influencing a single subsequent one, such as a soundbar conditioned on the purchase of either a television or a gaming console. A tree structure (right) models a primary choice that branches into multiple decisions, such as booking a flight that leads to choices for a hotel and a rental car. In all cases, customers may choose the no-purchase option at each stage, and impatient customers may exit the system entirely. This behavior is naturally captured by transitions to no-purchase options

The transition mechanism for any edge (U, W) generalizes our two-category model. After selecting an item i_U from category U, the customer forms an initial attraction to some j_W in W, determined by the cross-category transition vector $\boldsymbol{\lambda}^{i_U} = (\lambda_{i_U, j_W})_{j_W \in \mathbf{N}_W^+}$. Once j_W is drawn, the subsequent choice in W is conditionally independent of i_U. If $j_W \in S_W^+$, it is purchased; otherwise, the customer substitutes among S_W^+ according to the within-category model ϕ_W, conditioned on initially preferring j_W. That is, the customer draws a ranking where j_W is placed first and then selects the highest ranked available product.

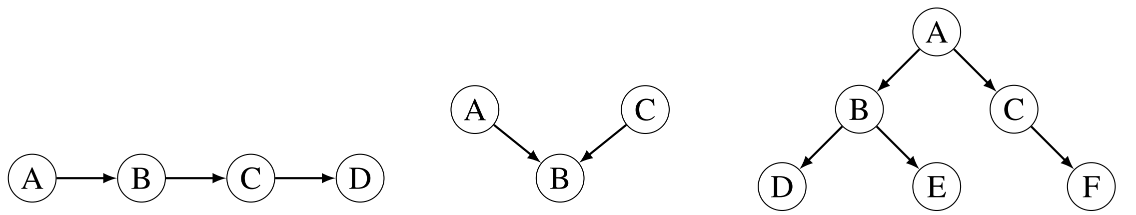


Figure 2 **Examples of cross-category dependency structures.**

3. Assortment Optimization

We now formulate the multi-category assortment optimization problem, where the goal is to jointly select assortments across categories to maximize total expected revenue. We begin with the two-category case, showing that the unconstrained problem can be solved efficiently when within-category choices follow MC models. We then extend the result to general DAG structures and establish the computational hardness of cardinality constrained assortment optimization.

3.1. Assortment Optimization for Two Categories

Consider first the two-category case. Let r_i^A and r_j^B denote the unit prices of product $i \in \mathbf{N}_A$ and $j \in \mathbf{N}_B$, with $r_{0_A}^A = r_{0_B}^B = 0$. The problem is to select $S_A \subseteq \mathbf{N}_A$ and $S_B \subseteq \mathbf{N}_B$ to maximize expected revenue:

$$\max_{S_A \subseteq \mathbf{N}_A, S_B \subseteq \mathbf{N}_B} \sum_{i \in S_A^+} \sum_{j \in S_B^+} (r_i^A + r_j^B) P(i, j, S_A, S_B), \tag{3}$$

where $P(i, j, S_A, S_B) = \phi_A(i, S_A)(\lambda_{i,j} + \sum_{\ell \in \mathbf{N}_B \setminus S_B} \lambda_{i,\ell} \phi_B(j, S_B | \ell))$ is given by Equation (1).

Recall that for general ranking-based choice models, even the single-category unconstrained assortment problem is NP-hard to approximate within any non-trivial factor (Aouad et al. 2018). We therefore focus on the setting where both ϕ_A and ϕ_B are MC models, for which the single-purchase assortment optimization problem is polynomial-time solvable (Blanchet et al. 2016). Extending to two categories is generally harder: the optimal assortment in one category can depend on the other. For previous MNL-based models that incorporate cross-category complementarity, the unconstrained optimization problem is NP-hard (Ke and Wang 2022, Chen et al. 2022, Tulabandhula et al. 2023). In contrast, our framework admits a polynomial-time algorithm even when both categories follow MC models.

Recall that ϕ_A and ϕ_B are defined by $(\boldsymbol{\psi}^A, \boldsymbol{\rho}^A)$ and $(\boldsymbol{\psi}^B, \boldsymbol{\rho}^B)$, respectively, and that $\boldsymbol{\lambda}^i$ denotes the transition probabilities from product $i \in \mathbf{N}_A$ to category B. Lemma 2 shows that conditional on i, the choice process in B is equivalent to an MC model $(\boldsymbol{\lambda}^i, \boldsymbol{\rho}^B)$. For notational simplicity, we denote this conditional model as $\phi_{B|i}$.

The key to solving the two-category assortment problem is to show that it can be decoupled. First, observe that if the optimal assortment in B were known, then computing the optimal assortment from A would reduce to a standard single-category assortment problem under MC with adjusted prices. Specifically, the price of any product i in A is augmented by the expected revenue from category B conditional on i being chosen from A, denoted by $R_i(S_B)$. This idea of using adjusted prices has been commonly used in multi-purchase models (Ke and Wang 2022, Chen et al. 2024). The main challenge is that computing the optimal assortment for B seems to require knowing optimal assortment for A, since the choice in A influences the initial attraction in B. Remarkably, our model breaks this dependency when ϕ_B is an MC model. The solution hinges on a crucial property of the MC choice model: for the unconstrained assortment problem, there exists an optimal assortment that is invariant to the initial arrival distribution. This 'invariant' optimal assortment depends on only the transition matrix and product prices. Such an invariant optimal assortment can be computed using the algorithms of Blanchet et al. (2016) or Désir et al. (2020); see Lemma 10 in Appendix B.2. In our framework, the choice i from category A affects only the arrival distribution in B (via $\boldsymbol{\lambda}^i$), while leaving the within-category transition matrix $\boldsymbol{\rho}^B$ unchanged. Consequently, the invariant optimal assortment for the MC model in category B with remains optimal for the joint problem, regardless of the assortments in A. This insight fully decouples the problem: the optimal assortment for B can be computed first, and the solution for A then follows by solving a single-category MC problem with adjusted prices. We now formalize this procedure.

Algorithm 1: Unconstrained Two-category Assortment Optimization

Input: Prices $(r_i^A)_{i\in\mathbf{N}_A^+}$ and $(r_j^B)_{j\in\mathbf{N}_B^+}$, choice models ϕ_A, ϕ_B, transition probability vectors $(\boldsymbol{\lambda}^i)_{i\in\mathbf{N}_A^+}$;

Compute the invariant optimal unconstrained assortment S_B^{ALG} for category B under $\phi_{B|1}$;

for $i \in \mathbf{N}_A^+$ **do**

  Compute the expected revenue from category B:
  $R_i(S_B^{\mathrm{ALG}}) \leftarrow \sum_{j\in S_B^{\mathrm{ALG}}} r_j^B \phi_{B|i}(j, S_B^{\mathrm{ALG}})$;

  Define adjusted price for product i: $r_i' \leftarrow r_i^A + R_i(S_B^{\mathrm{ALG}})$;

Compute the optimal unconstrained assortment S_A^{ALG} under ϕ_A using $(r_i')_{i\in\mathbf{N}_A^+}$ as prices;

Return: S_A^{ALG} and S_B^{ALG}.

The algorithm first computes the invariant optimal assortment for B, denoted by S_B^{ALG}. Since this assortment is independent of the initial arrival probabilities, we can use an arbitrary initial arrival probabilities; for concreteness, the algorithm uses $\boldsymbol{\lambda}^1$ in $\phi_{B|1}$. The invariant optimal assortment can be obtained in polynomial time using the iterative algorithms of Blanchet et al. (2016) (Algorithm 1) or Désir et al. (2020) (Algorithm 1). Importantly, these procedures do not depend on the initial arrival distribution, so the solution they output is invariant to the arrival probabilities. Note that not all optimal unconstrained assortments of an MC model are invariant, see Example 1 in Appendix B.1.

Given S_B^{ALG}, the algorithm then computes an adjusted price r_i' for each $i \in \mathbf{N}_A^+$ by adding the base price r_i^A to the expected revenue from category B, $R_i(S_B^{\mathrm{ALG}})$. Finally, it solves the unconstrained assortment optimization for category A under ϕ_A with adjusted prices, yielding S_A^{ALG}. A subtlety here is that the outside option 0_A may have a positive price, which is different from the standard assortment optimization setting where the price of outside option is 0. We address this by applying a simple price-shifting transformation that subtracts r_{0_A}' from all adjusted prices to make the outside option have zero price. We show this transformation does not change the optimal solution, see Lemma 11 in Appendix B.3. Thus we can use standard polynomial-time MC assortment optimization algorithms as in Blanchet et al. (2016), Feldman et al. (2021), Désir et al. (2020).

We now state the main result.

THEOREM 1. *For any Markov chain choice models ϕ_A and ϕ_B, Algorithm 1 computes an optimal solution to the problem* (3) *in polynomial time.*

Proof. Let $R(S_A, S_B)$ denote the total expected revenue given assortments (S_A, S_B). Let (S_A^*, S_B^*) be an optimal solution to (3), and $(S_A^{\mathrm{ALG}}, S_B^{\mathrm{ALG}})$ denote the output of Algorithm 1. We first show the optimality of $(S_A^{\mathrm{ALG}}, S_B^{\mathrm{ALG}})$ and then show the algorithm runs in polynomial time.

First, consider the subproblem for category B, assuming a fixed optimal assortment $S_A = S_A^*$ for category A. In this case, from (3), S_B^* is the optimal solution of the following problem:

$$\max_{S_B \subseteq \mathbf{N}_B} \sum_{j \in S_B^+} \sum_{i \in S_A^{*,+}} \phi_A(i, S_A^*) \phi_{B|i}(j, S_B) r_j^B.$$

We can define an aggregated choice model for category B as $\phi_{B|S_A^*}(j, S_B) = \sum_{i \in S_A^{*,+}} \phi_A(i, S_A^*) \phi_{B|i}(j, S_B)$. Since each $\phi_{B|i}$ is an MC model with the same transition matrix ρ^B but different initial arrivals, their convex combination is also an MC model with transition matrix $\boldsymbol{\rho}^B$ and a new initial arrival distribution given by $\boldsymbol{\psi}^{S_A^*} = \sum_{i \in S_A^{*,+}} \phi_A(i, S_A^*) \boldsymbol{\lambda}^i$. Thus the subproblem is the standard unconstrained assortment optimization for MC with parameters $(\boldsymbol{\psi}^{S_A^*}, \boldsymbol{\rho}^B)$. A key property of MC choice models is the existence of an invariant optimal assortment, which is optimal regardless of the initial probability distribution $\boldsymbol{\psi}$ (see Lemma 10 in Appendix B.2). Algorithm 1 computes this invariant assortment, which we denote by S_B^{ALG}. Since S_B^{ALG} is optimal for any initial distribution, it must also be optimal for the specific distribution $\boldsymbol{\psi}^{S_A^*}$ induced by S_A^*. This implies its expected revenue is at least as high as S_B^*: $\sum_{j \in S_B^{\mathrm{ALG}}} \sum_{i \in S_A^{*,+}} \phi_A(i, S_A^*) \phi_{B|i}(j, S_B^{\mathrm{ALG}}) r_j^B \geq \sum_{j \in S_B^*} \sum_{i \in S_A^{*,+}} \phi_A(i, S_A^*) \phi_{B|i}(j, S_B^*) r_j^B$. Therefore, considering the total expected revenue, we have our first key inequality:

$$R(S_A^*, S_B^{\mathrm{ALG}}) \geq R(S_A^*, S_B^*) \tag{4}$$

Next, we fix the assortment for category B to be S_B^{ALG}. The problem of finding the best assortment for category A then reduces to:

$$\max_{S_A \subseteq \mathbf{N}_A} \sum_{i \in S_A^+} (r_i^A + R_i(S_B^{\mathrm{ALG}})) \phi_A(i, S_A),$$

where $R_i(S_B^{\mathrm{ALG}}) = \sum_{j \in S_B^{\mathrm{ALG}}} r_j^B \phi_{B|i}(j, S_B^{\mathrm{ALG}})$ is the expected downstream revenue from category B if product i is chosen in category A. This is an unconstrained assortment optimization problem under choice model ϕ_A with adjusted prices $r_i^A + R_i(S_B^{\mathrm{ALG}})$ for $i \in \mathbf{N}_A^+$. Let S_A^{ALG} denotes the optimal solution for this problem. Then we have $R(S_A^{\mathrm{ALG}}, S_B^{\mathrm{ALG}}) \geq R(S_A^*, S_B^{\mathrm{ALG}})$. Combining with (4) yields $R(S_A^{\mathrm{ALG}}, S_B^{\mathrm{ALG}}) \geq R(S_A^*, S_B^*)$. Since (S_A^*, S_B^*) is an optimal solution, this proves that $(S_A^{\mathrm{ALG}}, S_B^{\mathrm{ALG}})$ is also optimal for the joint problem (3).

Finally, we analyze the runtime. The algorithm computes S_B^{ALG} in polynomial time via known MC assortment algorithms, performs $O(n_A)$ iterations of polynomial-time revenue calculations, and then solves the assortment problem for A in polynomial time. Hence the overall runtime is polynomial. □

REMARK 1 (GENERALIZATION BEYOND MC MODELS). The optimality result in Theorem 1 can be generalized. The choice model for category A, ϕ_A, need not be an MC model. Our decoupling approach remains optimal as long as the unconstrained assortment problem under ϕ_A can be solved in polynomial time (as is the case, for example, with the nested logit model). Furthermore, if an α-approximation algorithm exists for the problem under ϕ_A, the decoupling algorithm yields an α-approximate solution for the two-category problem. However, if the choice model for category B is tractable but does not have Markovian property, such as the nested logit model, our invariance-based decoupling argument does not apply, and the tractability of the joint optimization problem remains an open question.

REMARK 2 (EXTENSION TO PERSONALIZATION SETTING). Our framework also extends to the *personalization* setting, where the assortment for category B is determined after observing the customer's choice from category A. In this setting, the assortment problem in the two categories decouples naturally. Specifically, for each potential choice $i \in \mathbf{N}_A^+$, we solve for the optimal conditional assortment in category B, denoted $S_{B,i}^{\mathrm{ALG}}$. Then, for category A, the adjusted price for each product i becomes $r'_i = r_i^A + \sum_{j \in S_{B,i}^{\mathrm{ALG}}} r_j^B \, \phi_{B|i}(j, S_{B,i}^{\mathrm{ALG}})$. Notably, the optimality of this procedure does not require ϕ_B to be an MC model; it only requires that the single-category assortment optimization problems under ϕ_A and ϕ_B are tractable.

3.2. Assortment Optimization for a General DAG

The Markovian structure of the dependencies between categories enables our algorithm to extend to any general DAG. Because the choice process in each category W depends only on the selection made in its immediate predecessors, we do not need to track the customer's full purchase history. This memoryless property allows us to solve the problem via backward induction, starting from the terminal categories.

We formalize this backward induction using a dynamic programming approach over the dependency graph $G = (\mathcal{V}, \mathcal{E})$. The categories are processed in reverse topological order (i.e., each category is visited only after all its successors have been processed), ensuring that when we solve the subproblem for any category, the invariant optimal assortments for all its descendant categories have already been computed. The maximum expected revenue from choosing product i_U and continuing optimally through all of its descendant categories serves as the product's adjusted price. This value is calculated recursively using the following Bellman equation:

$$r'_{i_U} = r^U_{i_U} + \sum_{W \in \text{Succ}(U)} \left(\max_{S_W \subseteq \mathbf{N}_W} \sum_{i_W \in S^+_W} \phi_{W|i_U}(i_W, S_W) r'_{i_W} \right) \tag{5}$$

where Children(U) is the set of children of U, and any terminal category K (a category with no children) is simply $r_K(i_K)' = r^K_{i_K}$ for all $i_K \in \mathbf{N}^+_K$.

Crucially, this dynamic program is tractable when each category's choice model ϕ_W is an MC model. The inner maximization in the Bellman equation is a single-category assortment problem for category W with a given set of adjusted prices $\{r'_{i_W}\}$. As established previously, there exists an optimal assortment S^*_W for this subproblem that is invariant to the initial arrival distribution. Since the preceding choice i_U only influences the initial arrivals for $\phi_{W|i_U}$, we can find this invariant optimal assortment S^*_W and compute the value of the subproblem without needing to know the choice probabilities within category U. This decoupling at each step ensures the Bellman recursion can be solved efficiently. The full procedure is formalized in Algorithm 2 in Appendix B.4.

REMARK 3 (GENERALIZATION BEYOND MC MODEL). While our result assumes that each category follows an MC model, the approach can be generalized. Let $\mathcal{V}_r \subseteq \mathcal{V}$ denote the set of all root categories, where we define 'root categories' as those with no incoming edges in the DAG. Root categories represent the starting points of a customer's purchasing path. For example, in the convergent structure shown in Figure 2 (middle), both categories A and C are root categories. This distinction is important because the MC model assumption can be relaxed for root nodes. More precisely, our backward induction still computes an optimal solution in polynomial time under the following conditions: (i) Every non-root category ($U \in \mathcal{V} \setminus \mathcal{V}_r$) follows an MC model; and (ii) The unconstrained assortment problem for every root category ($U \in \mathcal{V}_r$) is solvable in polynomial time, even if its choice model is not an MC model. More generally, if the assortment problem for each root category U admits an α_U-approximation algorithm, our procedure yields a solution with an overall approximation factor of $\min_{U \in \mathcal{V}_r} \alpha_U$.

3.3. Cardinality Constrained Assortment Optimization

We now analyze the assortment optimization problem under cardinality constraints, which limit the number of distinct products that can be offered in an assortment. We consider the case where all non-root categories follow an MC model, while the root categories may follow more general choice models. In this section, we show that the problem remains tractable if constraints are limited to the root categories, but becomes computationally hard if they are applied throughout the graph.

3.3.1. Constraints on Root Categories We first consider the setting where a cardinality constraint applies only to the root categories of the DAG. This models many practical scenarios, such as offering a limited set of flights (the primary, root products) with a full range of ancillary services (the complementary, downstream add-ons). In this case, our backward induction approach remains effective. The algorithm is modified only at each root category, where a cardinality-constrained subproblem is solved using the adjusted prices propagated from downstream. If the choice models in the root categories admit a polynomial-time constant-factor approximation algorithm , we can still obtain a constant-factor approximation for the overall problem.

THEOREM 2. *Consider the multi-category assortment problem with cardinality constraints applied only to the root categories $\mathcal{V}_r$. Suppose that for each root category $U \in \mathcal{V}_r$, the cardinality-constrained single-category assortment problem under its choice model admits a polynomial-time α_U-approximation algorithm. Then the overall problem can be solved in polynomial time with an approximation factor of* $\min_{U \in \mathcal{V}_r} \alpha_U$.

As an immediate corollary, if each root category's cardinality-constrained assortment problem is polynomial-time solvable (i.e., $\alpha_U = 1$), then the overall problem can also be solved optimally in polynomial time. This is the case, for example, if all root categories follow the MNL choice model, for which the cardinality-constrained assortment problem is known to be solvable in polynomial time (Rusmevichientong et al. 2010).

3.3.2. Constraints on All Categories The problem becomes significantly more difficult when cardinality constraints are imposed on all categories. In this fully constrained setting, the key invariance property of the MC model breaks down: the optimal assortment for a downstream category now depends on the initial attraction probabilities, which are determined by choices in upstream categories. This interdependence prevents the use of our efficient backward induction algorithm and leads to computational intractability.

THEOREM 3. *There is a constant $c > 0$ such that, assuming Exponential Time Hypothesis (ETH), there is no $\Omega(g^{-1/(\log\log g)^c})$-approximation algorithm for the multi-category assortment problem with cardinality constraints on all categories, where g is the total number of products.*

4. Parameter Estimation

The section develops an estimation procedure for our model framework. We begin with the case of two categories where substitution within each category is captured by an MNL model, as this case preserves the core cross-category complementarity and highlights the main estimation challenges.

Let $\Theta = (\boldsymbol{\lambda}, \mathbf{v}^A, \mathbf{v}^B)$ denote the full set of model parameters. Let $\mathcal{H} = \{(S_A^t, S_B^t, a^t, b^t)\}_{t\in[T]}$ be the purchase history from T customers, where (S_A^t, S_B^t) are the offered assortments and (a^t, b^t) are the corresponding choices from $S_A^{t,+}$ and $S_B^{t,+}$. Based on the choice probabilities from Lemma 1, the observed-data log-likelihood function is:

$$\log L(\Theta;\mathcal{H}) = \sum_{t=1}^{T}\left[\log\left(\frac{v_{a^t}^A}{V^A(S_A^t)+1}\right) + \log\left(\lambda_{a^t,b^t} + \frac{v_{b^t}^B}{V^B(S_B^t)+1}\sum_{m\in\mathbf{N}_B\setminus S_B^t}\lambda_{a^t,m}\right)\right] \tag{6}$$

The terms involving $\mathbf{v}^A$ are decoupled from $(\boldsymbol{\lambda}, \mathbf{v}^B)$ and correspond to a standard MNL likelihood; thus, $\mathbf{v}^A$ can be estimated separately by maximizing a standard MNL likelihood function. However, the log-likelihood is not jointly concave in the remaining parameters $(\boldsymbol{\lambda}, \mathbf{v}^B)$, as shown in Appendix C. This non-concavity prevents the use of standard convex optimization methods. We therefore develop an Expectation-Maximization (EM) algorithm, which has been widely used to estimate choice models such as the Markov chain choice model or the general ranking-based choice models (van Ryzin and Vulcano 2017, Şimşek and Topaloglu 2018).

The EM algorithm introduces latent variables for the customer's unobserved initial interest in category B. Let X_m^t be an indicator that is 1 if the customer in transaction t was initially interested in product $m \in \mathbf{N}_B^+$, and 0 otherwise. The core idea is to construct a complete-data log-likelihood function by assuming these latent variables, $\mathbf{X} = \{X_m^t\}_{m\in\mathbf{N}_B^+, t\in[T]}$, are known, such that the new objective function is concave in the parameters $(\boldsymbol{\lambda}, \mathbf{v}^B)$.

We now derive this complete-data log-likelihood. After a customer chooses a^t from $\mathbf{N}_A^+$, their initial interest transitions to a product $m \in \mathbf{N}_B^+$ with probability $\lambda_{a^t,m}$. If we knew m, the logic is straightforward: if m is available ($m \in S_B^{t,+}$), the final choice must be m; if m is unavailable ($m \notin S_B^{t,+}$), the customer substitutes and chooses product j with probability $\frac{v_j^B}{V^B(S_B^t)+1}$, based on the derivation from Lemma 1. The complete-data log-likelihood, $\log L_C(\Theta;\mathcal{H},\mathbf{X})$, is therefore:

$$\begin{aligned}\log L_C(\Theta;\mathcal{H},\mathbf{X}) = \sum_{t=1}^{T}\Bigg\{&\log\left(\frac{v_{a^t}^A}{V^A(S_A^t)+1}\right) + \\ &\sum_{m\in\mathbf{N}_B^+} X_m^t \log\left(\lambda_{a^t,m}\left(\mathbb{1}\{m=b^t\} + \mathbb{1}\{m\in\mathbf{N}_B\setminus S_B^t\}\frac{v_{b^t}^B}{V^B(S_B^t)+1}\right)\right)\Bigg\}.\end{aligned}$$

The EM algorithm iteratively alternates between an Expectation (E) step and a Maximization (M) step to find parameters that maximize the observed-data likelihood. We assume the parameters lie in a compact set defined as: $\mathcal{P} = \{(\boldsymbol{\lambda}, \mathbf{v}^A, \mathbf{v}^B) \in \Delta^{(n_A+1)\times(n_B+1)} \times [0,C]^{n_A} \times [0,C]^{n_B}\}$ for a sufficiently large constant $C \in \mathbb{R}_+$. Starting with an initial estimate $\Theta^{(0)}$, the algorithm proceeds as follows:

Step 1 (Initialization). Choose initial estimates $\Theta^{(0)} = (\boldsymbol{\lambda}^{(0)}, \mathbf{v}^{A,(0)}, \mathbf{v}^{B,(0)}) \in \mathcal{P}$ and set the iteration counter $l = 0$.

Step 2 (E-step). For each transaction t and product $m \in \mathbf{N}_B^+$, compute the conditional expectation of the latent variable given the observed data and current parameter estimations: $\hat{X}_m^{t(l)} = \mathbb{E}[X_m^t | \mathcal{H}, \Theta^{(l)}]$.

Step 3 (M-step). Update the parameters by maximizing the expected complete-data log-likelihood over the feasible region $\mathcal{P}$: $\Theta^{(l+1)} = \arg\max_{\Theta \in \mathcal{P}} \mathbb{E}[\log L_C(\Theta; \mathcal{H}, \mathbf{X}) | \mathcal{H}, \hat{\mathbf{X}}^{(l)}]$. Increment $l \leftarrow l+1$ and return to Step 2. The process is repeated until the change in the observed log-likelihood or the parameters falls below a predefined tolerance.

We provide the detailed derivations for the E-step and M-step in Appendix C.2 and show that each step can be computed efficiently. Furthermore, the sequence of log-likelihood values generated by the EM algorithm is non-decreasing and converges to a finite limit. Any limit point of the parameter sequence is a stationary point of the observed-data likelihood function. As is common with EM algorithms, however, this stationary point is not guaranteed to be the global optimum. The result is stated in the following theorem, with proof in Appendix C.3.

THEOREM 4. *Let $\{\Theta^{(l)} = (\boldsymbol{\lambda}, \mathbf{v}^{A,(l)}, \mathbf{v}^{B,(l)}) : l = 1, 2, \ldots\}$ be the sequence of parameter estimates generated by the EM algorithm. Then the log-likelihood is non-decreasing, $L(\Theta^{(l+1)}) \geq L(\Theta^{(l)})$ for $l \geq 1$, and $L(\Theta^{(l)})$ converges to $L(\Theta^*)$ for some stationary point Θ^*.*

Generalizations of the estimation framework. Our EM-based estimation framework can be generalized beyond the initial setting of two MNL models and two categories. Its modular design handles more general choice models and multi-category structures arranged in a DAG, as we detail in Appendix C.4. The key idea is to introduce edge-specific latent variables and leverage the likelihood's modularity to decouple the M-step updates for each choice model and transition probability.

5. Synthetic Data Experiments

This section evaluates the performance of our proposed model using synthetic data. Our objective is to compare our model with established benchmarks in a controlled environment where the ground truth is known. Specifically, we focus on assessing the model's ability to capture varying degrees of cross-category complementarity and whether improved modeling accuracy translates into better assortment decisions. We complement this section with real-world case studies in Section 6.

5.1. Experimental Design

We begin by describing the data generation process, the models used for comparison, and the evaluation metrics.

5.1.1. Ground Truth and Data Generation We describe the ground-truth customer choice model that captures complex dependencies and then describe the data generation process.

Choice model construction. Our ground-truth model is based on ranking-based choice models. We use this model to simulate complex real-world choice behavior. We consider two product categories, A and B, with $n_A = 10$ and $n_B = 8$ products, respectively. For category A, customer preferences are characterized by $m_A = 10$ customer classes, and each class k has an arrival probability α_k^A, generated by sampling values β_k independently from a uniform distribution $U[0,1]$ and then normalizing: $\alpha_k^A = \beta_k / \sum_{\kappa=1}^{m_A} \beta_\kappa$. Product rankings for each customer class k in category A follow a procedure adapted from Aouad et al. (2023). We assume products are indexed in decreasing baseline preferences. For each customer class k, we define a consideration set by sampling a random interval $Q_k = [i_L, \ldots, i_U]$. Within each consideration set, the baseline rankings are perturbed by independent Gaussian noise and then re-sorted to obtain the final product ranking σ_k^A. To further simulate effects like brand preference or non-consideration, we also randomly remove products from each class's final ranking with a probability $p_{\text{del}} = 0.2$.

For category B, we use a similar rank-based construction, extended to incorporate cross-category complementarity. We generate $m_B = 10$ baseline rankings $\{\sigma_k^0\}_{k=1}^{m_B}$ and arrival probabilities $\{\psi_k^B\}_{k=1}^{m_B}$ using the same procedure as for category A. Complementarity is introduced by perturbing the ranking σ_k^0 based on the product $i \in \mathbf{N}_A$ chosen from A. For each product $j \in \mathbf{N}_B^+$, we sample $\epsilon_{ij} \sim \mathcal{N}(0,1)$ and define a score $s_{ij} = \sigma_k^0(j) + \theta\epsilon_{ij}$, where $\theta \geq 0$ controls the strength of complementarity. Sorting $\{s_{ij}\}_{j \in \mathbf{N}_B^+}$ in non-decreasing order yields the conditional ranking σ_k^i of products in category B conditional on purchasing i. When $\theta = 0$, the ranking reduces to the baseline ranking, and choices in category B are independent of the choice in A. As θ increases, the conditional ranking becomes more dependent on the selected product from category A. The probability of choosing product $j \in \mathbf{N}_B^+$ from an offered assortment S_B, given the prior choice of i, is then determined by these conditional rankings: $\sum_{k=1}^{m_B} \psi_k^B \mathbb{1}\{j = \arg\min_{\ell \in S^+} \sigma_k^i(\ell)\}$.

Transaction data simulation. To ensure our results are robust, we perform 10 independent replications of the entire experiment. Each replication consists of the following steps. First, we create a new ground-truth model for category A using the procedure described above. Then, keeping the category A model fixed, we generate ten corresponding models for category B by setting the complementarity parameter θ to 11 distinct values, ranging from 0.0 (no complementarity) to 5.0 (strong complementarity). This procedure results in a total of $11 \times 10 = 110$ unique ground-truth model configurations. For each model configuration, we simulate a dataset of $12,000$ transactions. In each transaction, an assortment for each category is drawn uniformly at random from the power set of its products ($\mathcal{P}(\mathrm{N}_A)$ and $\mathcal{P}(\mathrm{N}_B)$). A customer's choice is then generated from the corresponding ground-truth model. This process yields 110 distinct datasets.

5.1.2. Models for Comparison For the synthetic experiments, we use the MNL-based specification of our model, denoted MARKOVMNL and detailed in Section 2. Although the ground-truth data are generated from a more general ranking-based model, we adopt the MNL specification for the following reasons. First, it allows for a fair comparison with existing MNL-based benchmarks that capture complementarity. Second, this model is a special case of our general framework. If it performs well, the general model, which is more flexible, is expected to perform even better. Third, the MNL-based model is the most convenient to estimate and demonstrates practical value in implementation. Indeed, the MNL model remains one of the most widely used discrete choice models in both academic research and industrial practice (Shi 2015, Feldman et al. 2022), even though choice behavior in these settings may be more complex. We compare our model against the following benchmarks:

- MULTIMNL: The two-category MNL model from Ke and Wang (2022), which was introduced in Section 2.1. Recall that in this model, choices in category A induce a mixture of MNLs on category B, making it a highly expressive model. Finding the optimal assortment for this model requires solving a mixed-integer linear program (MILP).
- INDMNL: A baseline using two independent MNL models, one for each category. This model assumes no complementarity across categories, and its optimal assortment can be computed efficiently with the revenue-ordered optimal structure Talluri and Van Ryzin (2004). Recall that INDMNL is a special case of both MARKOVMNL and MULTIMNL, while MULTIMNL and MARKOVMNL cannot be reduced to one another.

Parameter estimation. For each of the 110 datasets, we perform a $70\% - 30\%$ random split to create training and test sets. On the training data, we estimate the parameters for our MARKOVMNL model using the EM algorithm from Section 4, which terminates when the change in average log-likelihood or the maximum parameter deviation between iterations falls below a threshold of 10^{-2}. The benchmark models, MULTIMNL and INDMNL, are estimated by directly maximizing their respective likelihood functions since the likelihood functions are concave.

5.1.3. Evaluation Metrics We evaluate the performance of all trained models on the test sets. Unless otherwise specified, each metric is calculated for a specific value of θ by averaging the outcomes from the 10 independent replications. Since all models use the same MNL specification for category A, the estimated model in category A is identical across all methods. As our evaluation of model fit and prediction accuracy relies solely on the estimated parameters, we focus on performance in category B, conditional on the choice in category A. For optimal assortment evaluation, however, we compute the joint optimal assortments for both categories A and B.

Model fit and predictive accuracy. We use three metrics to evaluate how well each model explains customer behavior:

- **Log-likelihood:** The average total log-likelihood of the model on the test set.
- **Top-K hit rate:** Conditioned on choice in category A, the proportion of transactions where the customer's chosen product in category B was among the K products with the highest predicted probability from the model for a given K.
- **Rank accuracy:** The average rank of the product actually purchased by the customer, where ranks are determined by sorting predicted choice probabilities in descending order. Lower values indicate better performance.

These metrics are commonly used in related literature and highlight distinct aspects of model fit and predictive accuracy: log-likelihood measures overall model fit, the top-K hit rate offers a practical measure of predictive power, and rank accuracy provides a nuanced view of how well the model prioritizes the chosen product.

Assortment optimization performance. To assess the economic value of each model, we evaluate the quality of its assortment decisions. For each estimated model, we solve for its optimal unconstrained assortment and then evaluate that assortment's expected revenue under the known ground-truth choice model. This provides a direct measure of each model's practical impact.

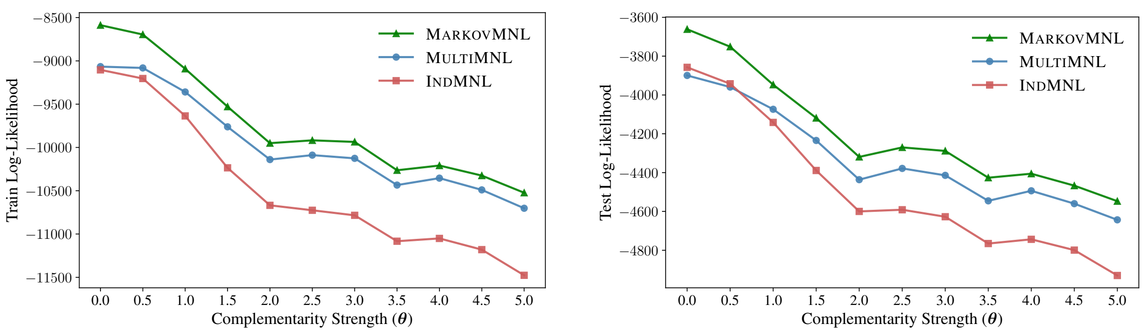
5.2. Results

For conciseness, we present the key experimental trends graphically in the main text. The detailed numerical results corresponding to each figure are tabulated in Appendix D.

Model fit evaluation. We first evaluate model fit using in-sample (training) and out-of-sample (test) log-likelihoods. As shown in Figure 3, our proposed model, MARKOVMNL consistently achieves the highest log-likelihood across all levels of complementarity. This outperformance stems from different strengths relative to each benchmark.

The comparison with INDMNL, which ignores cross-category effects, confirms our model's ability to capture cross-category complementarity. The performance gap between MARKOVMNL and INDMNL grows with the complementarity parameter θ. When $\theta = 5.0$, the test log-likelihood for INDMNL is 8.42% lower than that of MARKOVMNL.

The comparison with MULTIMNL reveals a different trend. While our model consistently outperforms MULTIMNL across all values of θ, the magnitude of this advantage is largest when complementarity is weak and narrows as θ increases. This trend stems from the structural differences between the two models. At $\theta = 0$ (no complementarity), MULTIMNL reduces to a standard MNL model. Our MARKOVMNL model, however, simplifies to a special case of MC choice model that can subsume the standard MNL (See Appendix A.2 for details). This greater inherent flexibility allows our model to better fit the choice behavior when θ is small. As θ increases, both our model and MULTIMNL capture the complementarity, but use distinct structures and recall that neither model subsumes the other. This causes the initial advantage of MARKOVMNL to narrow.



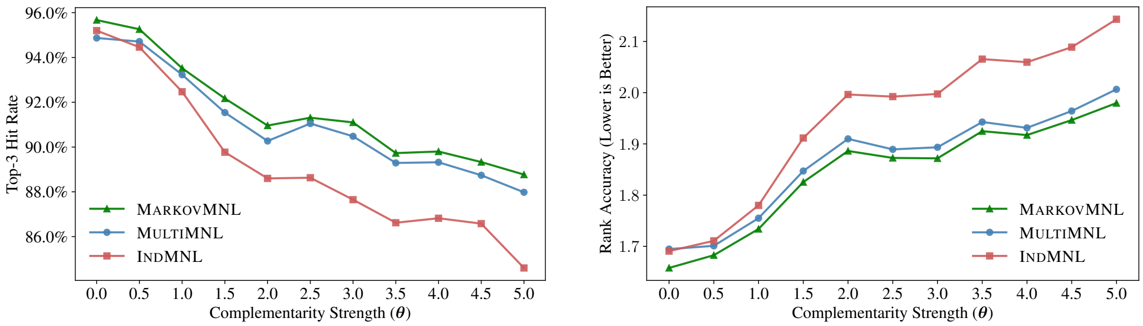
(a) Performance on training set

(b) Performance on test set

Figure 3 Comparison of model fit

Prediction accuracy evaluation. We next evaluate prediction accuracy using top-3 hit rates and rank accuracy. As shown in Figure 4, these metrics confirm the findings from the log likelihood analysis. The INDMNL model, which ignores complementarity, performs well only when $\theta = 0$. Its hit rate falls sharply as complementarity strengthens, dropping by 4.70 percentage points (p.p.) relative to our model when θ is large. In all scenarios, MARKOVMNL maintains the highest hit rate of the three models.

The rank accuracy results follow a similar pattern. This metric represents the average rank of the product purchased (with ranks determined by sorting predicted probabilities); lower values indicate better performance. As shown in Figure 4(b), MARKOVMNL achieves the best (lowest)



(a) top-3 Hit Rate

(b) Rank Accuracy

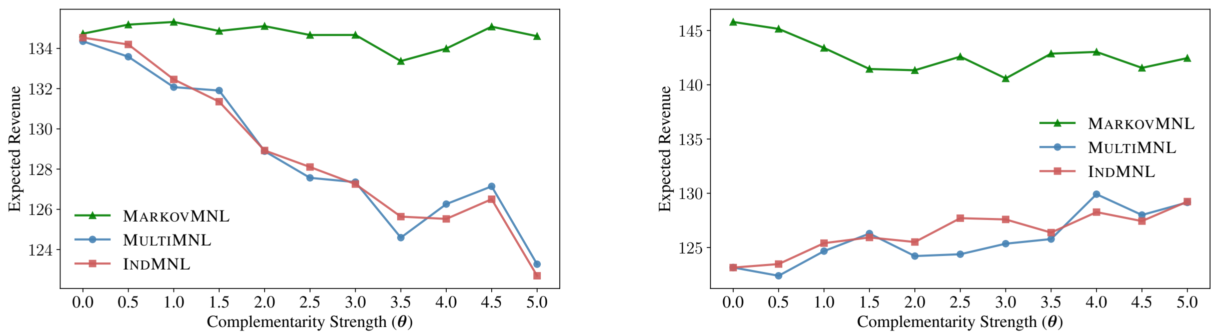
Figure 4 **Comparison of top-3 hit rate and rank accuracy.**

average rank in all scenarios. IndMNL again shows a significant weakness as complementarity increases. While MultiMNL improves upon IndMNL, it is consistently outperformed by our model. Both metrics thus confirm that MarkovMNL more accurately predicts customer choices, and its advantage is particularly pronounced relative to models that do not account for product complementarity.

Expected revenue from optimal assortments. To evaluate the economic value of the models, we compare the expected revenue from the optimal assortments they recommend. We construct four test scenarios by combining two distinct market structures with two different price distributions (Normal and Uniform) to ensure our findings are robust. All reported revenues are averaged over 50 independent price generation trials for each scenario. The two market structures are defined by how a product's price relates to its index k, and recall that baseline customer preference is highest for products with a low index k when we construct the ranking-based model.

1. **Low Price Sensitivity**: Price aligns with preference, reflecting a quality-focused market. Lower-indexed (more preferred) products have higher revenues, which decrease with k: $r_k \sim \max\{\mathcal{N}(100-5k, 25), 0.1\}$ or $r_k \sim \mathcal{U}[5-0.5k, 10-0.5k]$ under a uniform distribution.
2. **High Price Sensitivity**: Price opposes preference, reflecting a price-sensitive market. Higher-indexed (less preferred) products have higher revenues, which increase with k: $r_k \sim \max\{\mathcal{N}(50+5k, 25), 0.1\}$, or $r_k \sim \mathcal{U}[5+0.5k, 10+0.5k]$.

For brevity, we focus our discussion on results when the prices follow Normal distributions (Figure 5). The results for the Uniform distribution are qualitatively similar and are provided in Appendix D.1.2. In the high price sensitivity setting, the results show a clear revenue advantage for our MarkovMNL model as complementarity strengthens. When complementarity is absent ($\theta = 0$), the performance of all models is similar. However, as its strength increases, our model again achieves the highest expected revenue. Compared to MULTIMNL, the performance advantage is particularly significant when considering computational cost. In the low price sensitivity setting, our model consistently outperforms the benchmarks, with revenue gains of up to 15.63%.



(a) High price sensitivity (b) Low price sensitivity

Figure 5 Comparison of expected revenue under the Normal price distribution.

Summary of synthetic experiment results. Synthetic experiments show that the MARKOVMNL model consistently outperforms the INDMNL and MULTIMNL benchmarks. Our model achieves superior model fit and higher predictive accuracy, and this advantage that widens as product complementarity (θ) increases. This improved accuracy leads to more profitable assortment decisions, increasing expected revenue across a wide range of market conditions. By contrast, INDMNL risks large revenue losses when complementarity is strong, while MULTIMNL relies on a computationally expensive MILP for optimization. Therefore, MARKOVMNL provides a more robust and practical tool for assortment planning.

6. Case Studies With Real World Data

In the previous section, we conducted synthetic experiments to evaluate our model under systematically varying complementarity strength. Here, we use real-world transaction data to address the following questions: (i) Does meaningful complementarity exist across product categories in retail settings, and if so, what is its magnitude? (ii) For category pairs exhibiting such complementarity, how does our proposed model perform against established benchmarks? (iii) Can our model uncover actionable managerial insights about product-level interactions?

To answer these questions, we first introduce a metric to quantify complementarity at the category level and use it to identify high-signal category pairs. We also introduce another metric to evaluate product-level interactions. Next, we evaluate model performance on selected pairs and compare fit and predictive accuracy. In addition, we introduce a second metric to quantify the strength of complementarity between specific products, which we use to extract interpretable, product-level insights. Finally, we demonstrate the framework's flexibility by extending the analysis to a three-category setting.

6.1. Data and Preprocessing

We use a dataset from a joint project between Stanford and UC Berkeley, which has been used in prior literature such as Che et al. (2012), Ruiz et al. (2019). It contains $5,968,528$ purchases of $5,590$ products from $3,206$ customers over 97 weeks from a major grocery store. More information can be found at `https://are.berkeley.edu/SGDC`. We randomly partition the data into a 70% training set and a 30% test set.

The raw transaction data requires several preprocessing steps to prepare for choice model estimation. First, a common challenge in retail data is that the offered assortment for each transaction is unobserved. To address this, we follow the standard approach of inferring the offered set from products purchased within a given time period, as discussed by Jagabathula and Rusmevichientong (2019) and Mitrofanov et al. (2024). Specifically, for each week, we define the available assortment as the set of all unique products purchased by any customer during that period. Second, if there are multiple purchases in a single category, we decompose each transaction into distinct choice observations. For instance, a transaction with purchases a_1, a_2 from category A and b_1 from category B are purchased, is mapped to two observations: (a_1, b_1) and (a_2, b_1).

Next, we narrow our analysis to transactions with at least one purchase from the first category. This is necessary because we cannot distinguish customers who considered but rejected all products in a category from those who ignored the category entirely. With this filtering, we can naturally model the conditional choice behavior in the second category and observe no-purchase events in that category. While some no-purchase customers in those transactions may not be actively interested in the second category (e.g., they already have enough of those products at home), we assume that all of them consider products from both categories. Finally, to ensure robust model estimation, we restrict the ground set to the set of products that appear in at least 10% of transactions with purchases in their respective category.

6.2. Metrics for Quantifying Complementarity

To quantify the strength and nature of cross category effects, we develop and use two distinct metrics. The first is an *Aggregate Complementarity Metric (CM)*, which is a data-driven measure used to identify categories with significant complementarity effects from raw transaction data. The second is a *Specific Complementarity Score (SCS)*, which is a model-based measure derived from estimated parameters to provide interpretable insights into product-level interactions.

Aggregate Complementarity Metric (CM) for Screening This metric is designed to distinguish true, heterogeneous complementarity from simple, homogeneous co-occurrence. A heterogeneous effect implies that the choice of a specific product in one category influences the choice of a specific product in another. In contrast, a homogeneous effect, such as in the classic 'beer and diapers' case, reflects a correlation driven by shopper demographics rather tha product interactions (i.e., the choice of a specific beer brand does not affect the preference for a specific diaper brand).

To capture this distinction, the CM metric measures how much the purchase distribution in category B deviates when conditioned on the purchase of a specific product $i \in \mathbf{N}_A$. Let $c(i,j)$ be the count of transactions where product $i \in \mathbf{N}_A^+$ and product $j \in \mathbf{N}_B^+$ are purchased together. For this metric, we assume all products in $\mathbf{N}_B$ are shown to each customer. Thus the empirical conditional probability of purchasing j given a purchase of i is: $\hat{P}(j|i) = \frac{c(i,j)}{\sum_{k \in \mathbf{N}_B^+} c(i,k)}$. We compare this to the aggregate unconditional purchase probability of j, calculated as: $\hat{P}(j) = (\sum_{i' \in \mathbf{N}_A^+} c(i',j))/(\sum_{k \in \mathbf{N}_B^+} \sum_{i' \in \mathbf{N}_A^+} c(i',k))$. For each product $i \in \mathbf{N}_A^+$, we measure the deviation of its conditional purchase distribution from the aggregate purchase probability distribution using the L_1 norm: $d(i) = \sum_{j \in \mathbf{N}_B^+} |\hat{P}(j|i) - \hat{P}(j)|$. The final metric is the weighted average of these deviations, where f_i is the total number of transactions in which product $i \in \mathbf{N}_A^+$ was selected:

$$\text{CM} = \sum_{i \in \mathbf{N}_A^+} \frac{f_i}{\sum_{k \in \mathbf{N}_A^+} f_k} d(i).$$

The CM score is bounded between 0 and 2, as it represents a weighted L_1 distance between probability distributions. A score of $\text{CM} = 0$ occurs when $P(j|i) = \bar{P}(j)$ for all $i \in \mathbf{N}_A^+, j \in \mathbf{N}_B^+$, indicating that the choice in category B is completely decoupled from the specific choice in category A. In such a scenario, our model would reduce to two independent choice models. This property allows the metric to filter out the false identification of co-occurrence as complementarity. For example, in the classic 'beer and diapers' case, the co-purchase is driven by shopper demographics rather tha product-level interactions. This homogeneous effect would yield a low CM score.

Conversely, a higher score indicates stronger complementarity. To validate this, we computed CM scores on our synthetic data and real data. Figure 6 shows that the CM score increases monotonically with our ground-truth complementarity parameter, θ, before plateauing at $\theta \approx 7.0$. This result confirms that CM is a valid tool for measuring the strength of cross-category complementarity. Table 1 shows the CM scores for several category pairs, illustrating a low score for pairs with homogeneous co-occurrence (e.g., Diapers and Beer) and progressively higher scores for those with stronger interactions (e.g., Cake Mix and Cake Frosting). Subsequently, we use this metric to screen for category pairs with strong complementarity effects in the real-world dataset.

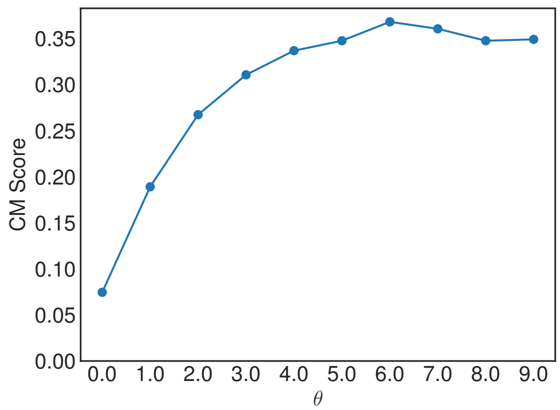


Figure 6 **CM versus ground-truth complementarity parameter θ on synthetic data.**

Category A	**Category B**	**CM**
diaper	beer	0.0712
coffee	creamer	0.0738
milk/yogurt	granola	0.1303
pasta	pasta sauce	0.2593
patties/franks	buns	0.4202
cake mix	cake frosting	0.5844

Table 1 **CM scores for selected category pairs in real data.**

Specific Complementarity Score (SCS) for Interpretation To explain the interaction between individual products, we introduce the Specific Complementarity Score (SCS), $\tilde{\lambda}_{ij}$, which is derived from the parameters of our estimated model.

After estimating our model, the parameter $\tilde{\lambda}_{ij}$ captures the lift that purchasing product i gives to product j. We define the SCS as: $\tilde{\lambda}_{ij} = \lambda_{ij} - \frac{v_j^B}{\sum_{k \in \mathbf{N}_B} v_k^B + 1}$. This calculation isolates the specific interaction effect (λ_{ij}) by subtracting a baseline influence derived from the product's intrinsic utility within category B. A score of $\tilde{\lambda}_{ij} \approx 0$ implies no specific complementarity, while positive or negative scores suggest that purchasing product i makes product j more or less attractive, respectively.

6.3. Model Evaluation and Interpretability on Real Data

We now evaluate our model on several combinations of categories with high CM scores. Our goal is to compare model performance and illustrate the interpretability of our model's estimates. For evaluation, we use the same metrics as in the synthetic data experiments: log-likelihood, top-3 hit rates, and rank accuracy. However, real-world data introduces a challenge not present in the synthetic setting: the proportion of no-purchase outcomes is typically high. Thus, we introduce an Effective Hit

Rate (E-HR) to measure prediction accuracy on actual purchases while excluding the influence of the no-purchase option. The E-HR measures top-1 prediction accuracy conditioned on a purchase being made in category B. Let $\mathcal{T}_B = \{t : b^t \in \mathbf{N}_B\}$ be the set of transactions with a purchase in category B, where b^t is the chosen product. Let $\hat{p}_t(j)$ denote the model's predicted probability of choosing product j in transaction t, and recall that $S_B^t \subseteq \mathbf{N}_B$ denotes the inferred assortment for category B in transaction t. The E-HR is then defined as: E-HR $= \frac{1}{|\mathcal{T}_B|} \sum_{t \in \mathcal{T}_B} \mathbb{1}\{\arg\max_{j \in S_B^t} \hat{p}_t(j) = b^t\}$, where $\hat{p}_t(j)$ is the model's predicted probability for choosing product j.

Example 1: Cake Mixes and Cake Frostings. We first consider cake mixes as category A (29 products) and cake frosting as category B (31 products). The CM score for this pair is 0.5844, indicating significant complementarity. This score is notably high, as it is higher than other pairs in the real dataset (Table 1) and also higher than the maximum value of approximately 0.35 observed in our synthetic experiments (Figure 6). This pair is also known to have strong complementarity from previous literature (Manchanda et al. 1999, Sinitsyn 2012).

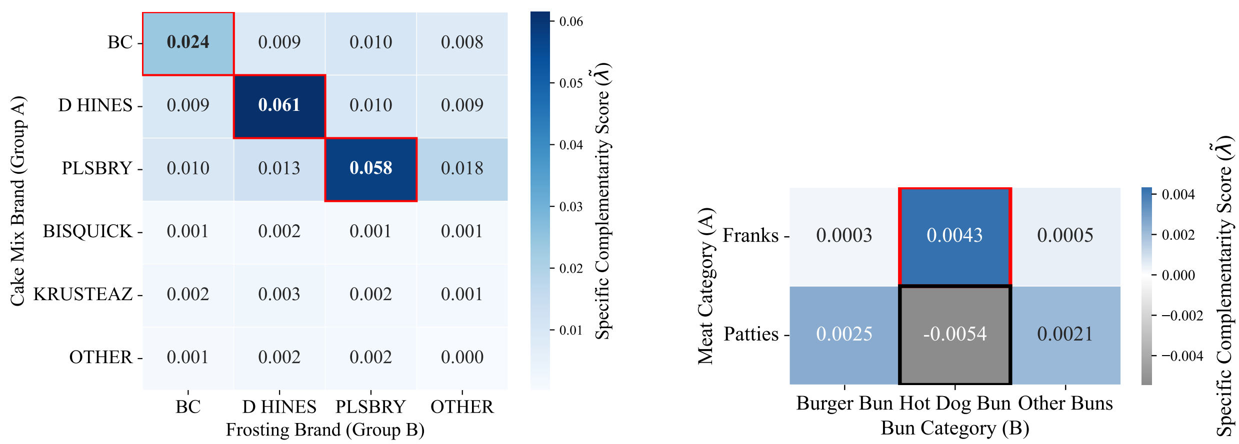
Table 2 shows that both MarkovMNL and MultiMNL models yield substantial improvements over IndMNL across all metrics. Specifically, our MarkovMNL improves the in-sample log-likelihood (LL) by 18.66% and the out-of-sample LL by 14.57%. In terms of prediction, it achieves a 4.86 percentage point (p.p.) increase in the top-3 Hit Rate and a 9.87 p.p. increase in the Effective Hit Rate (E-HR). The rank accuracy for MarkovMNL also improves significantly, with the mean rank decreasing by 16.26%. These results highlight the critical importance of modeling complementarity for this category pair. While both MultiMNL and our MarkovMNL model achieve comparable improvements over IndMNL in model fit and predictive performance, MarkovMNL offers a key advantage: its corresponding assortment optimization problem remains polynomial-time solvable, whereas the problem under MultiMNL is NP-hard.

Table 2 Model fit and prediction accuracy for cake mixes and cake frostings Percentage improvements are relative to IndMNL. For HR and EHR, parenthetical values are absolute differences in percentage points (p.p.).

Model	In-Sample LL	Out-of-Sample LL	top-3 HR	E-HR	Rank Acc.
IndMNL	-36896.34	-15936.90	72.26%	7.18%	3.71
MultiMNL	-30129.69 (+18.34%)	-13513.76 (+15.20%)	77.14% (+4.88 p.p.)	17.11% (+9.93 p.p.)	3.11 (-16.10%)
MarkovMNL	-30013.26 (+18.66%)	-13614.58 (+14.57%)	77.12% (+4.86 p.p.)	17.05% (+9.87 p.p.)	3.11 (-16.26%)

Beyond predictive accuracy, we analyze insights into specific product-level interactions based on $\tilde{\lambda}$. We aggregate these scores by brand to explore the market structure, visualizing the results in

Figure 7(a). The heatmap reveals a strong brand-matching effect: the on-diagonal scores, representing the lift within major brands like Betty Crocker, Duncan Hines, and Pillsbury, are significantly larger than the near-zero off-diagonal scores. The Pillsbury-to-Pillsbury interaction, for instance, yields the highest lift ($\tilde{\lambda} = 0.058$). This pattern aligns with intuitive consumer behavior, where shoppers prefer brand consistency, thus empirically validates that our model indeed captures realistic, brand-level market dynamics. These findings offer actionable insights for retailers; for instance, a retailer could use this knowledge to guide targeted promotions, such as creating brand-specific bundles (e.g., ”Buy a Pillsbury cake mix, get 25% off Pillsbury frosting”) to increase basket size.



(a) Complementarity heatmap for cake mixes and frostings.

(b) Complementarity heatmap for meats and buns.

Figure 7 Product-level complementarity heatmaps ($\tilde{\lambda}$).

Example 2: Meats and Buns. Our second case study investigates the classic pairing of meats (category A: beef patties, franks, etc.; 34 products) and buns (category B: hamburger, hot dog, etc.; 21 products). This pair has a CM score of 0.4202, indicating substantial, though slightly less pronounced, complementarity compared to our first example.

Table 3 confirms that modeling complementarity again yields significant gains. Compared to INDMNL, our MARKOVMNL model improves the out-of-sample log likelihood by 5.93% and shows clear benefits in predictive accuracy. For instance, the top-3 Hit Rate increases by 2.84 percentage points and the Effective Hit Rate by 4.73 percentage points, while rank accuracy improves by over 12%. These improvements confirm the value of our approach for pairs with varying degrees of complementarity.

We next analyze the Specific Complementarity Scores ($\tilde{\lambda}$) between meat subcategories (‘franks’, ‘patties’) and bun subcategories (‘hot dog buns’, ‘burger buns’). The results, shown in Figure 7(b),

Table 3 Model fit and prediction accuracy for meats and buns. For LL and rank accuracy, parenthetical values are relative improvements over INDMNL. For HR and EHR, they are absolute differences in percentage points (p.p.).

Model	In-Sample LL	Out-of-Sample LL	top-3 HR	E-HR	Rank Acc.
INDMNL	-51063.85	-21689.80	73.53%	26.22%	4.06
MULTIMNL	-46633.42 (+8.68%)	-20241.67 (+6.68%)	76.31% (+2.78 p.p.)	30.93% (+4.71 p.p.)	3.57 (-12.07%)
MARKOVMNL	-46450.70 (+9.03%)	-20403.12 (+5.93%)	76.37% (+2.84 p.p.)	30.95% (+4.73 p.p.)	3.56 (-12.32%)

reveal highly intuitive consumption patterns. Franks exhibit a strong positive complementarity with hot dog buns ($\tilde{\lambda} = 0.0043$), while patties pair most strongly with burger buns ($\tilde{\lambda} = 0.0025$). Interestingly, the model also captures anti-complementarity: patties have a negative score with hot dog buns ($\tilde{\lambda} = -0.0054$), indicating that buying a beef patty makes a customer less likely to be interested in a hot dog bun. This demonstrates the model's ability to learn not just positive pairings but also logical mismatches from transaction data.

REMARK 4 (SCALABILITY TO MULTIPLE CATEGORIES). Our framework can be extended to settings with more than two product groups. To demonstrate this scalability, we analyzed a three-group sequential choice model ($A \to B \to C$) based on a 'Meats $\to$ Buns $\to$ Condiments' case study. The results confirm the advantage of our approach in capturing complex, multi-stage dependencies. The MARKOVMNL model provides a substantially better model fit, improving the out-of-sample log-likelihood by over 10% relative to a category-independent model and 5% better than MULTIMNL. The performance of our model and MULTIMNL on other predictive metrics is comparable, both improving upon INDMNL. The detailed experimental setup and full results are presented in Appendix D.2.

7. Conclusion

In this paper, we develop a sequential multi-purchase choice framework that links product categories through Markovian dependencies. Our framework represents the relationship between product categories as a DAG and allows for a general choice model within each category, capturing both cross-category complementarity and within-category substitution. By conditioning each downstream choice on the product selected in the previous category, the model captures cross-category complementarity while preserving the tractability that retailers may need for assortment optimization. We derive a polynomial-time algorithm for the unconstrained assortment problem that extends from two groups to any DAGs, and propose a scalable EM algorithm for estimation.

Our experiments, using both synthetic and large-scale retail data, highlight the significant value of this approach. On synthetic data, we show that our model yields substantial gains in model fit and predictive accuracy, which translates to revenue gain of over $6\% - 10\%$. Using a large grocery dataset, we introduce a metric to quantify complementarity and identified specific product-level interactions, such as a brand-matching effect between cake mix and frosting. These findings provide several managerial insights. First, complementarity is significant even in routine purchases, and optimizing assortments for it can materially improve margins. Second, managers can use our framework to identify high-potential category pairs and discover product-level interactions. These insights not only help improve expected revenue from assortment optimization, but also provide information for targeted cross-selling, joint promotions, or optimized shelf placement. Finally, we demonstrate that for sequential purchases, tractable models can effectively capture complex cross-category interactions.

There are several interesting directions for future work. First, while our work focuses on the unconstrained assortment problem, there remains scope for developing practically useful heuristics for the cardinality-constrained version. Second, a natural extension is the joint optimization of assortments and prices, though a major challenge here is the need for a high-quality transaction dataset with sufficient price variation. Finally, a mixture of our model could capture complementarity in both directions for each edge in the DAG and even model symmetric complementarity. How to solve the assortment optimization problem under this model is a challenge problem.

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Appendix A: Omitted Details and Proofs in Section 2

A.1. Invariance of MNL Probabilities Under Conditioning

LEMMA 3. *Let $\mathbf{N}$ be a ground set and $S \subseteq \mathbf{N}$ an assortment. Assume a ranking-based choice model ϕ is equivalent to an MNL model with preference weights $\{v_j\}_{j\in\mathbf{N}}$. If we condition on the ranking starting with an unavailable product $k \in \mathbf{N}\setminus S$, then the conditional choice probability $\phi(i,S \mid k)$ is independent of k, and is given by*

$$\phi(i,S \mid k) \;=\; \frac{v_i}{1+\sum_{j\in S} v_j} \;=\; \phi(i,S).$$

Proof of Lemma 3. The proof proceeds in two parts. First, we construct a ranking distribution equivalent to the MNL model. We show that this ranking model yields the same choice probabilities as those in the standard MNL model without conditioning. Next, we verify that conditioning on an unavailable top product leaves these probabilities unchanged.

We first construct the ranking-based choice model equivalent to an MNL model with weights $\{v_j\}_{j\in\mathbf{N}}$. Recall that $v_0 = 1$ for the outside option, and set $\mathbf{N}^+ := \mathbf{N}\cup\{0\}$. Rankings are generated sequentially. Given a prefix $P \subseteq \mathbf{N}^+$ of already-ranked products, the next product x is drawn from the set of unranked products $\mathbf{N}^+\setminus P$ with probability

$$\Pr[\text{next product is } x \mid \text{prefix is } P] = \frac{v_x}{\sum_{m\in\mathbf{N}^+\setminus P} v_m}.$$

This process defines a probability θ_σ for each complete ranking σ.

We next show that this ranking model produces the standard MNL choice probabilities for any assortment S. A customer's choice is the first element of $S^+ := S\cup\{0\}$ that appears in the ranking. This occurs after a (possibly empty) prefix P of products from outside the assortment, i.e., $P \subseteq \mathbf{N}\setminus S$. Consider any step before a choice has been made and let $U := \mathbf{N}^+\setminus P$ be the set of unranked products. Then, for $i \in S$,

$$\frac{\Pr[\text{next is } i \mid U]}{\Pr[\text{next is } 0 \mid U]} = \frac{v_i/\sum_{m\in U} v_m}{1/\sum_{m\in U} v_m} = v_i.$$

This ratio is independent of the set of unavailable products U (and thus independent of the prefix P). Since the final choice probabilities are aggregated over all such valid sequences, these probabilities share the same constant ratio:

$$\phi(i,S) = v_i\phi(0,S) \text{ for all } i \in S.$$

Since the choice probabilities for all products must sum to 1, we have $\sum_{i\in S^+}\phi(i,S) = 1$. Thus,

$$\phi(0,S) + \sum_{i\in S}\phi(i,S) = \phi(0,S) + \sum_{i\in S} v_i\,\phi(0,S) = 1,$$

so $\phi(0,S) = \frac{1}{1+\sum_{i\in S} v_j}$ and hence $\phi(i,S) = \frac{v_i}{1+\sum_{i\in S} v_j}$.

Finally, consider conditioning on the ranking starting with a specific unavailable product $k \in \mathbf{N}\setminus S$. The key observation is that, after k is ranked first, the conditional model is equivalent to being constructed by applying the same sequential process and the same weights on all remaining products. Therefore, the same odds argument gives

$$\phi(i,S \mid k) = v_i\,\phi(0,S \mid k) \qquad \text{and} \qquad \phi(0,S \mid k) = \frac{1}{1+\sum_{j\in S} v_j},$$

for all products $i \in S^+$ and $S \subseteq \mathbf{N}\setminus\{k\}$. This yields $\phi(i,S \mid k) = \frac{v_i}{1+\sum_{j\in S} v_j} = \phi(i,S)$. $\square$

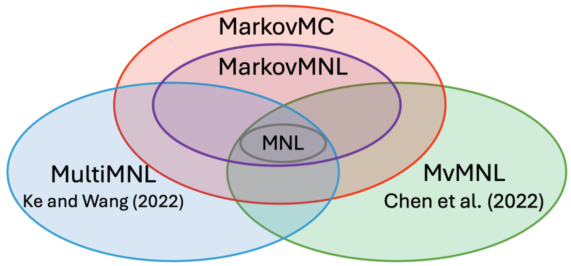


Figure 8 A Venn diagram illustrating the relationships between the choice models.

A.2. Relationship Between Two-Category Choice Models

In this section, we compare our two-category model with the related models in Ke and Wang (2022) and Chen et al. (2022). Recall that we use MARKOVMC and MARKOVMNL to denote our model with MC and MNL as special cases, respectively. Figure 8 visualizes the relationships between all related models. We first formally define the choice models in Ke and Wang (2022) and Chen et al. (2022). We use MULTIMNL to denote the sequential MNL choice model from Ke and Wang (2022). In this model, a customer first chooses a product i from the first-category assortment S_A according to an MNL model with preference weights $\{w_i\}_{i\in\mathbf{N}_A}$. Conditional on choosing i, the customer chooses from S_B according to a distinct MNL model with parameters $\{w_{i,j}\}_{j\in\mathbf{N}_B}$. A key feature is that each choice $i\in\mathbf{N}_A^+$ induces its own set of preference parameters for the second stage. Without loss of generality, $w_{0_A}=w_{i,0_B}=1$ for all $i\in\mathbf{N}_A^+$. The probability of choosing $i\in S_A$ and $j\in S_B$ is:

$$P_{\text{MULTIMNL}}(i,j,S_A,S_B)=\frac{w_i}{\sum_{k\in S_A}w_k+1}\frac{w_{i,j}}{\sum_{\ell\in S_B}w_{i,\ell}+1}.$$

We use MVMNL to denote the multivariate MNL model from Chen et al. (2022). In this model, each bundle (i,j) for $i\in\mathbf{N}_A^+$ and $j\in\mathbf{N}_B^+$ has a single utility parameter $u_{i,j}$. The preference weight of the no-purchase option is set to $u_{0_A,0_B}=1$. The probability of choosing bundle (i,j) from assortments S_A and S_B is:

$$P_{\text{MVMNL}}(i,j,S_A,S_B)=\frac{u_{i,j}}{\sum_{k\in S_A^+}\sum_{l\in S_B^+}u_{k,l}}.$$

A core property of this model is that the odds of choosing bundle (i,j) over (k,l), given by $u_{i,j}/u_{k,l}$, are independent of the offered assortment, provided that all products are included in the assortments.

Comparison with Ke and Wang (2022)

LEMMA 4. *The* MARKOVMNL *model class and the* MULTIMNL *model class are distinct; neither model class contains the other.*

Proof of lemma 4. We prove this by constructing counterexamples in both directions.

*(*MARKOVMNL $\not\subset$ MULTIMNL*).* Consider a universe with $\mathbf{N}_A=\{1\}$ and $\mathbf{N}_B=\{2,3\}$. Let the MARKOVMNL parameters be $\lambda_{1,2}=\lambda_{1,3}=1/3$ and $v^B_{0_B}=v^B_2=1, v^B_3=2$. (We omit parameters related to the first-stage no-purchase option 0_A as they are not needed here).

Conditional on purchasing product 1 from category A, the choice probabilities for products in category B are:

- For assortment $S_B=\{2,3\}$: $P_{\text{MARKOVMNL}}(2,S_B|1)=\lambda_{1,2}=\frac{1}{3}$ and $P_{\text{MARKOVMNL}}(3,S_B|1)=\lambda_{1,3}=\frac{1}{3}$.

- For assortment $S_B = \{2\}$: $P_{\text{MarkovMNL}}(2, S_B|1) = \lambda_{1,2} + \lambda_{1,3}\frac{v_2^B}{v_2^B+1} = \frac{1}{3} + \frac{1}{3}\cdot\frac{1}{2} = \frac{1}{2}$.
- For assortment $S_B = \{3\}$: $P_{\text{MarkovMNL}}(3, S_B|1) = \lambda_{1,3} + \lambda_{1,2}\frac{v_3^B}{v_3^B+1} = \frac{1}{3} + \frac{1}{3}\cdot\frac{2}{3} = \frac{5}{9}$.

For a MULTIMNL model to match these probabilities, its parameters $\{w_{1,j}\}$ must satisfy:

- From $S_B = \{2,3\}$: $\frac{w_{1,2}}{w_{1,2}+w_{1,3}+1} = \frac{1}{3}$ and $\frac{w_{1,3}}{w_{1,2}+w_{1,3}+1} = \frac{1}{3}$, which implies $w_{1,2} = w_{1,3}$.
- From $S_B = \{2\}$: $\frac{w_{1,2}}{w_{1,2}+1} = \frac{1}{2}$, which gives $w_{1,2} = 1$.
- From $S_B = \{3\}$: $\frac{w_{1,3}}{w_{1,3}+1} = \frac{5}{9}$, which gives $w_{1,3} = \frac{5}{4}$.

These conditions imply a contradiction that $w_{1,2} = w_{1,3}$ and $w_{1,2} \neq w_{1,3}$. Thus, no MULTIMNL model can represent this MARKOVMNL instance.

(MultiMNL $\not\subset$ MarkovMNL). Consider a universe with $\mathbf{N}_A = \{1,2\}$ and $\mathbf{N}_B = \{3,4\}$. Let the MULTIMNL parameters be $w_{1,3} = 2$, $w_{1,4} = M$ (for some constant $M > 0$), and $w_{2,3} = w_{2,4} = w_{2,0_B} = w_{1,0_B} = 1$.

To represent this instance with a MARKOVMNL model, we first match the choice probabilities when the full assortment $S_B = \{3,4\}$ is offered. This determines the required $\boldsymbol{\lambda}$ parameters by equating them with the MULTIMNL probabilities:

$$\begin{aligned}
\lambda_{13} &= P_{\text{MultiMNL}}(3, \{3,4\}|1) = \frac{w_{1,3}}{w_{1,3}+w_{1,4}+1} = \frac{2}{M+3},\\
\lambda_{14} &= P_{\text{MultiMNL}}(4, \{3,4\}|1) = \frac{w_{1,4}}{w_{1,3}+w_{1,4}+1} = \frac{M}{M+3},\\
\lambda_{23} &= P_{\text{MultiMNL}}(3, \{3,4\}|2) = \frac{w_{2,3}}{w_{2,3}+w_{2,4}+1} = \frac{1}{3},\\
\lambda_{24} &= P_{\text{MultiMNL}}(4, \{3,4\}|2) = \frac{w_{2,4}}{w_{2,3}+w_{2,4}+1} = \frac{1}{3}.
\end{aligned}$$

Now, consider the smaller assortment $S_B = \{3\}$. The MULTIMNL probabilities are $P_{\text{MultiMNL}}(3, \{3\}|1) = \frac{w_{1,3}}{w_{1,3}+1} = \frac{2}{3}$ and $P_{\text{MultiMNL}}(3, \{3\}|2) = \frac{w_{2,3}}{w_{2,3}+1} = \frac{1}{2}$. For the MARKOVMNL model to match these, its parameters must satisfy:

$$\begin{aligned}
P_{\text{MarkovMNL}}(3, \{3\}|1) &= \lambda_{13} + \lambda_{14}\frac{v_3^B}{v_3^B+1} = \frac{2}{3},\\
P_{\text{MarkovMNL}}(3, \{3\}|2) &= \lambda_{23} + \lambda_{24}\frac{v_3^B}{v_3^B+1} = \frac{1}{2}.
\end{aligned}$$

Substituting the λ values we derived:

$$\begin{aligned}
\frac{2}{M+3} + \frac{M}{M+3}\frac{v_3^B}{v_3^B+1} &= \frac{2}{3},\\
\frac{1}{3} + \frac{1}{3}\frac{v_3^B}{v_3^B+1} &= \frac{1}{2}.
\end{aligned}$$

The second equation implies $v_3^B = 1$. Plugging $v_3^B = 1$ into the first equation gives $\frac{2}{M+3} + \frac{M}{2(M+3)} = \frac{2}{3}$, which yields $M = 0$. This contradicts the requirement that $M > 0$. Therefore, no MARKOVMNL model can represent this MULTIMNL instance. □

Comparison with Chen et al. (2022)

LEMMA 5. *The* MARKOVMNL *model class and the* MVMNL *model class are distinct; neither model class contains the other.*

Proof of Lemma 5. *(MarkovMNL $\not\subset$ MvMNL).* The key intuition here is that our model can violate the IIA property for bundles in MvMNL. Consider a universe with $\mathbf{N}_A = \{1\}$ and $\mathbf{N}_B = \{2, 3\}$. Set the MarkovMNL parameters to $\lambda_{0_A,2} = \lambda_{0_A,3} = \lambda_{1,2} = \lambda_{1,3} = \frac{1}{3}$ and $v^B_{0_B} = v^B_2 = 1, v^B_3 = 2$. Let $S_A = \{1\}$. For simplicity, assume the choice probability of product 1 from category A is $\phi_A(1, \{1\}) = P_1$.

- When the full assortment $S_B = \{2, 3\}$ is offered, the choice probabilities in MarkovMNL models are $P_{\text{MarkovMNL}}(1, 2, S_A, S_B) = \lambda_{1,2}P_1 = \frac{1}{3}P_1$ and $P_{\text{MarkovMNL}}(1, 3, S_A, S_B) = \lambda_{1,3}P_1 = \frac{1}{3}P_1$. The odds ratio of these joint probabilities is 1. In an MvMNL model, this implies $u_{12}/u_{13} = 1$. Similarly, $u_{0_A,2}/u_{0_A,3} = 1$.
- When the assortment is restricted to $S_B = \{2\}$, the choice probability is $P_{\text{MarkovMNL}}(1, 2, S_A, S_B) = (\lambda_{1,2} + \lambda_{1,3}\frac{v^B_2}{v^B_2+1})P_1 = \frac{1}{2}P_1$. Similarly, for $S_B = \{3\}$, the conditional probability is $P_{\text{MarkovMNL}}(1, 3, S_A, S_B) = (\lambda_{1,3} + \lambda_{1,2}\frac{v^B_3}{v^B_3+1})P_1 = (\frac{1}{3} + \frac{1}{3} \cdot \frac{2}{3})P_1 = \frac{5}{9}P_1$. For an MvMNL model, since $u_{12} = u_{13}$ and $u_{0_A,2} = u_{0_A,3}$, $P_{\text{MvMNL}}(1, 3, S_A, S_B) = P_{\text{MvMNL}}(1, 2, S_A, S_B)$. Thus, this MarkovMNL instance cannot be represented by any MvMNL model.

(MvMNL $\not\subset$ MarkovMNL). Consider a universe with $\mathbf{N}_A = \{1\}$ and $\mathbf{N}_B = \{2, 3\}$. Let the MvMNL bundle utilities be $u_{1,2} = 2, u_{0_A,3} = 2$, and all other $u_{ij} = 1$.

First, we determine the $\boldsymbol{\lambda}$ parameters that a MarkovMNL model would require in order to match the conditional probabilities when the full assortment $S_A = \{1\}, S_B = \{2, 3\}$ is offered. We have the following choice probabilities from MvMNL:

$$
\begin{aligned}
P_{\text{MvMNL}}(2, S_B|1, S_A) &= \frac{u_{1,2}}{u_{1,2} + u_{1,3} + u_{1,0_B}} = \frac{2}{2+1+1} = \frac{1}{2}, \\
P_{\text{MvMNL}}(3, S_B|1, S_A) &= \frac{u_{1,3}}{u_{1,2} + u_{1,3} + u_{1,0_B}} = \frac{1}{4}, \\
P_{\text{MvMNL}}(2, S_B|0_A, S_A) &= \frac{u_{0_A,2}}{u_{0_A,2} + u_{0_A,3} + u_{0_A,0_B}} = \frac{1}{1+2+1} = \frac{1}{4}, \\
P_{\text{MvMNL}}(3, S_B|0_A, S_A) &= \frac{u_{0_A,3}}{u_{0_A,2} + u_{0_A,3} + u_{0_A,0_B}} = \frac{2}{4} = \frac{1}{2}.
\end{aligned}
$$

Any MarkovMNL representation would therefore require $\lambda_{12} = \frac{1}{2}$, $\lambda_{13} = \frac{1}{4}$, $\lambda_{02} = \frac{1}{4}$, $\lambda_{03} = \frac{1}{2}$. Now consider assortment $S_B = \{2\}$, from MvMNL, we have:

$$
\begin{aligned}
P_{\text{MvMNL}}(2, \{2\}|1, \{1\}) &= \frac{u_{1,2}}{u_{1,0_B} + u_{1,2}} = \frac{2}{3}, \\
P_{\text{MvMNL}}(2, \{2\}|0_A, \{1\}) &= \frac{u_{0_A,2}}{u_{0_A,0_B} + u_{0_A,2}} = \frac{1}{2}.
\end{aligned}
$$

To match the MarkovMNL model, we need

$$
\begin{aligned}
P_{\text{MarkovMNL}}(2, \{2\}|1, \{1\}) &= \lambda_{12} + \lambda_{13}\frac{v^B_2}{v^B_2 + 1} = \frac{1}{2} + \frac{1}{4}\frac{v^B_2}{v^B_2 + 1} = \frac{2}{3}. \\
P_{\text{MarkovMNL}}(2, \{2\}|0_A, \{1\}) &= \lambda_{0_A,2} + \lambda_{0_A,3}\frac{v^B_2}{v^B_2 + 1} = \frac{1}{4} + \frac{1}{2}\frac{v^B_2}{v^B_2 + 1} = \frac{1}{2}.
\end{aligned}
$$

No value of v^B_2 could satisfy both equations, so this MvMNL model cannot be represented by any MarkovMNL model. $\square$

Next, we show that MvMNL and MultiMNL cannot express each other, either.

Lemma 6. *The* MvMNL *model class and the* MultiMNL *model class are distinct; neither model class contains the other.*

Proof of Lemma 6. We construct a counterexample for each direction of inclusion.

*(*MvMNL $\not\subset$ MultiMNL*).* The intuition is that in the MultiMNL model, the choice from category A is independent of the assortment S_B in category B. We show that an MvMNL model can produce a instance where the marginal choice probability in category A does depend on S_B.

Consider a universe with $\mathbf{N}_A = \{1\}$ and $\mathbf{N}_B = \{2,3\}$, each with a no-purchase option $(0_A, 0_B)$. In an MvMNL model, set $u_{1,3} = 3$ and $u_{i,j} = 1$ for all other pairs $(i,j) \in \{0_A,1\} \times \{0_B,2,3\}$.

First, consider the assortment $S_A = \{1\}, S_B = \{2\}$. The set of available bundles is $\{(1,2),(1,0_B),(0_A,2),(0_A,0_B)\}$. All corresponding utilities are 1, so the total utility is 4. The bundle choice probabilities are all $\frac{1}{4}$. For a MultiMNL model to match, it must preserve the marginal choice probability ratio in category A:

$$\frac{P_{\text{MvMNL}}(\text{choose } 1)}{P_{\text{MvMNL}}(\text{choose } 0_A)} = \frac{P_{\text{MvMNL}}(1,2,S_A,S_B) + P_{\text{MvMNL}}(1,0_B,S_A,S_B)}{P_{\text{MvMNL}}(0_A,2,S_A,S_B) + P_{\text{MvMNL}}(0_A,0_B,S_A,S_B)} = \frac{1/4+1/4}{1/4+1/4} = 1.$$

This implies that the first-stage parameter must satisfy $w_1 = 1$, since we set the no-purchase preference weight to be 1.

Next, consider the assortment $S_A = \{1\}, S_B = \{3\}$. The available bundles are $\{(1,3),(1,0_B),(0_A,3),(0_A,0_B)\}$. The utilities are $\{3,1,1,1\}$, so the total utility is 6. The choice probabilities are $P(1,3,S_A,S_B) = 3/6$, $\phi(1,0_B,S_A,S_B) = 1/6$, $\phi(0_A,3) = 1/6$, and $\phi(0_A,0_B) = 1/6$. For a MarkovMNL model to match, the first-stage ratio must be:

$$\frac{P_{\text{MvMNL}}(\text{choose } 1)}{P_{\text{MvMNL}}(\text{choose } 0_A)} = \frac{P_{\text{MvMNL}}(1,3,S_A,S_B) + P_{\text{MvMNL}}(1,0_B,S_A,S_B)}{P_{\text{MvMNL}}(0_A,3,S_A,S_B) + P_{\text{MvMNL}}(0_A,0_B,S_A,S_B)} = \frac{3/6+1/6}{1/6+1/6} = \frac{4/6}{2/6} = 2.$$

This implies $w_1 = 2$, which contradicts the previous finding that $w_1 = 1$.

*(*MultiMNL $\not\subset$ MvMNL*).* Again, let $\mathbf{N}_A = \{1\}$ and $\mathbf{N}_B = \{2,3\}$. In a MultiMNL model, set $w_1 = w_{0_A} = w_{0_A,2} = w_{1,3} = 1$ and $w_{1,2} = w_{0_A,3} = 2$. Assume that the no-purchase preference weights $w_{0_A}, w_{1,0_B}, w_{0_A,0_B}$ are all set to 1.

First, consider the assortment $S_A = \{1\}, S_B = \{2\}$. The bundle probabilities are:

- $P_{\text{MultiMNL}}(1,0_B,S_A,S_B) = \frac{w_1}{w_1+1} \cdot \frac{1}{w_{1,2}+1} = \frac{1}{2} \cdot \frac{1}{3} = \frac{1}{6}$,
- $P_{\text{MultiMNL}}(0_A,0_B,S_A,S_B) = \frac{w_{0_A}}{w_1+w_{0_A}} \cdot \frac{1}{w_{0_A,2}+1} = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$.

For an MvMNL model to match this, the odds ratio between the no-purchase bundles $(1,0_B)$ and $(0_A,0_B)$ must be

$$\frac{u_{1,0_B}}{u_{0_A,0_B}} = \frac{P_{\text{MultiMNL}}(1,0_B,S_A,S_B)}{P_{\text{MultiMNL}}(0_A,0_B,S_A,S_B)} = \frac{1/6}{1/4} = \frac{2}{3}.$$

Next, consider the assortment $S_A = \{1\}, S_B = \{3\}$. The bundle probabilities involving no purchase in the second stage are:

- $P_{\text{MultiMNL}}(1,0_B,S_A,S_B) = \frac{w_1}{w_1+1} \cdot \frac{1}{w_{1,3}+1} = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$,
- $P_{\text{MultiMNL}}(0_A,0_B,S_A,S_B) = \frac{w_{0_A}}{w_1+w_{0_A}} \cdot \frac{1}{w_{0_A,3}+1} = \frac{1}{2} \cdot \frac{1}{3} = \frac{1}{6}$.

Thus, the odds ratio must be

$$\frac{u_{1,0_B}}{u_{0_A,0_B}} = \frac{P_{\text{MultiMNL}}(1,0_B,S_A,S_B)}{P_{\text{MultiMNL}}(0_A,0_B,S_A,S_B)} = \frac{1/4}{1/6} = \frac{3}{2}.$$

This contradicts the earlier ratio of $2/3$ derived from the first assortment. Therefore, no MvMNL model can represent this MultiMNL instance. $\square$

LEMMA 7. *The* MARKOVMC *model class and the* MULTIMNL *model class are distinct; neither model class contains the other.*

Proof of Lemma 7. *(*MARKOVMC$\not\subset$ MULTIMNL*).* We have shown that MARKOVMNL$\not\subset$ MULTIMNL in Lemma 4. Since MARKOVMNL is a special case of MARKOVMC, it follows that MARKOVMC$\not\subset$ MULTIMNL. It remains to show the reverse direction.

*(*MULTIMNL $\not\subset$ MARKOVMC*).* Consider a MULTIMNL choice model with preference weights $\{w_i\}_{i\in\mathbf{N}_A}$ and $\{w_{i,j}\}_{i\in\mathbf{N}_A^+,j\in\mathbf{N}_B}$. Suppose $\mathbf{N}_A=\{1\}$ and $\mathbf{N}_B=\{2,3\}$. Consider assortment $S_B=\{2\}$. To match this model, MARKOVMC needs to have $\lambda_{i,j}=\frac{w_{i,j}}{\sum_{j\in\mathbf{N}_B}v_{w,j}+1}$ for all $i\in\mathbf{N}_A^+$. Moreover, we need:

$$P_{\text{MarkovMC}}(2,\{2\}|0_A)=\lambda_{0_A,3}\boldsymbol{\rho}_{3,2}+\lambda_{0_A,2}=\frac{w_{0_A,2}}{w_{0_A,2}+1},$$
$$P_{\text{MarkovMC}}(2,\{2\}|1)=\lambda_{1,3}\boldsymbol{\rho}_{3,2}+\lambda_{1,2}=\frac{w_{1,2}}{w_{1,2}+1}.$$

Solving the first equation yields $\boldsymbol{\rho}_{3,2}=\frac{w_{0_A,2}}{w_{0_A,2}+1}$ while solving the second equation yields $\boldsymbol{\rho}_{3,2}=\frac{w_{1,2}}{w_{1,2}+1}$. When $w_{1,2}\neq w_{0,2}$, this is a contradiction. □

LEMMA 8. *The* MARKOVMC *and* MVMNL *model classes are distinct; neither contains the other.*

Proof of Lemma 8. *(*MARKOVMC$\not\subset$ MVMNL*).* We have shown in Lemma 5 that MARKOVMNL$\not\subset$ MVMNL. Since MARKOVMNL is a special case of MARKOVMC, it follows that MARKOVMC$\not\subset$ MVMNL.

*(*MVMNL$\not\subset$ MARKOVMC*).* Consider a MVMNL model with $\mathbf{N}_A=\{1\}$ and $\mathbf{N}_B=\{2,3\}$. Consider the assortments $S_A=\{1\}$ and $S_B=\{2\}$. For MARKOVMC to match this model, it would require

$$\lambda_{i,j}=\frac{v_{i,j}}{\sum_{j\in\mathbf{N}_B}v_{i,j}+1},\qquad\forall i\in\mathbf{N}_A^+,$$

and, moreover:

$$P_{\text{MarkovMC}}(2,\{2\}\mid 0_A,\{1\})=\lambda_{0_A,3}\,\boldsymbol{\rho}_{3,2}+\lambda_{0_A,2}=\frac{u_{0_A,2}}{u_{0_A,2}+1},$$
$$P_{\text{MarkovMC}}(2,\{2\}\mid 1,\{1\})=\lambda_{1,3}\,\boldsymbol{\rho}_{3,2}+\lambda_{1,2}=\frac{u_{1,2}}{u_{1,2}+1}.$$

The first equation implies $\boldsymbol{\rho}_{3,2}=\frac{u_{0_A,2}}{u_{0_A,2}+1}$, while the second implies $\boldsymbol{\rho}_{3,2}=\frac{u_{1,2}}{u_{1,2}+1}$. If $u_{1,2}\neq u_{0_A,2}$, these requirements are inconsistent, yielding a contradiction. □

LEMMA 9. MARKOVMNL *includes the independent MNL models as a special case.*

Proof of Lemma 9. We prove this in two parts: (i) any two independent MNL models can be represented by a MARKOVMNL model; (ii) the inclusion is strict, since some MARKOVMNL models cannot be represented by any standard MNL model.

For part (i), consider independent MNL models for categories A and B, with preference weights $\{u_i^A\}_{i\in\mathbf{N}_A}$ and $\{u_j^B\}_{j\in\mathbf{N}_B}$. The no-purchase weights for both categories are normalized to 1. We construct an equivalent MARKOVMNL model by setting $v_i^A=u_i^A$ for all $i\in\mathbf{N}_A$ and $v_j^B=u_j^B$ for all $j\in\mathbf{N}_B$. The key step is to define the transition probabilities as the MNL probabilities under the full assortment, independent of the first-stage choice i:

$$\lambda_{i,j}=\frac{u_j^B}{1+\sum_{k\in\mathbf{N}_B}u_k^B},\qquad\forall i\in\mathbf{N}_A^+.$$

Then, for any assortment $S_B \subseteq \mathbf{N}_B$, the probability of choosing $j \in S_B$ in the MARKOVMNL model, conditional on first-stage choice i, is

$$
\begin{aligned}
P_{\text{MarkovMNL}}(j, S_B \mid i, S_A) &= \lambda_{i,j} + \sum_{k \in \mathbf{N}_B \setminus S_B} \lambda_{i,k} \frac{v_j^B}{1 + \sum_{q \in S_B} v_q^B} \\
&= \frac{u_j^B}{1 + \sum_{m \in \mathbf{N}_B} u_m^B} + \sum_{k \in \mathbf{N}_B \setminus S_B} \frac{u_k^B}{1 + \sum_{m \in \mathbf{N}_B} u_m^B} \cdot \frac{u_j^B}{1 + \sum_{q \in S_B} u_q^B} \\
&= \frac{u_j^B}{1 + \sum_{q \in S_B} u_q^B}.
\end{aligned}
$$

This matches the standard MNL probability.

For part (ii), we give a counterexample. The key insight is that MARKOVMNL can violate the IIA property of standard MNL models. Consider $\mathbf{N}_A = \{1\}$, $\mathbf{N}_B = \{2, 3\}$, with parameters $\lambda_{1,2} = \lambda_{1,3} = 1/3$ and $v_{0_B}^B = v_2^B = 1$, $v_3^B = 2$. (Parameters related to the first-stage no-purchase option 0_A are omitted, as they are not needed here.)

Conditional on choosing product 1 from A, the choice probabilities in B are:

- $S_B = \{2, 3\}$: $P_{\text{MarkovMNL}}(2, S_B \mid 1, S_A) = 1/3$, $P_{\text{MarkovMNL}}(3, S_B \mid 1, S_A)) = \frac{1}{3}$.
- $S_B = \{2\}$: $P_{\text{MarkovMNL}}(2, S_B \mid 1, S_A)) = \frac{1}{2}$.
- $S_B = \{3\}$: $P_{\text{MarkovMNL}}(3, S_B \mid 1, S_A)) = \frac{5}{9}$.

For a standard MNL model to match these, its parameters $\{u_j^B\}_{j \in \mathbf{N}_B}$ must satisfy:

- $S_B = \{2, 3\}$: $\frac{u_2^B}{u_2^B + u_3^B + 1} = \frac{1}{3}$ and $\frac{u_3^B}{u_2^B + u_3^B + 1} = \frac{1}{3}$, implying $u_2^B = u_3^B$.
- $S_B = \{2\}$: $\frac{u_2^B}{u_2^B + 1} = \frac{1}{2}$, giving $u_2^B = 1$.
- $S_B = \{3\}$: $\frac{u_3^B}{u_3^B + 1} = \frac{5}{9}$, giving $u_3^B = \frac{5}{4}$.

These conditions imply both $u_2^B = u_3^B$ and $u_2^B \neq u_3^B$, a contradiction. Hence no standard MNL model can represent this MARKOVMNL instance. □

A.3. Connection to the Model of Cao et al. (2023)

Cao et al. (2023) propose a single-purchase model that is a mixture of an independent demand model and an MNL model. In their framework, a customer belongs to one of two segments. With probability $\tilde{\lambda} \in (0, 1)$, a customer belongs to the first segment and chooses product $i \in S$ with a fixed probability θ_i. With probability $1 - \tilde{\lambda}$, the customer is in the second segment and chooses according to a standard MNL model with weights $(v_j)_{j \in \mathbf{N}_B}$. The resulting choice probability for a product $i \in S$ is $\phi_{\text{MIX}}(i, S) = \tilde{\lambda}\theta_i + (1 - \tilde{\lambda}) \frac{v_i}{\sum_{k \in S} v_k + 1}$.

We now show that our model is structurally distinct from this mixture model. For a clear comparison, we consider a simplified version of our model with no complementarity, meaning the transition probabilities $\boldsymbol{\lambda}^i$ are identical for all choices $i \in \mathbf{N}_A^+$. We can thus write $\lambda_{i,j}$ as λ_j for simplicity.

First, our model cannot be reduced to the mixture model. In our simplified setting, the choice probability for a product $j \in S_B$ is given by: $(\sum_{i \in S_A^+} \phi_A(i, S_A))(\lambda_j + \sum_{\ell \in \mathbf{N}_B \setminus S_B} \lambda_\ell \frac{v_j^B}{\sum_{\ell \in S_B} v_l^B + 1}) = \lambda_j + \sum_{\ell \in \mathbf{N}_B \setminus S_B} \lambda_\ell \frac{v_j^B}{\sum_{\ell \in S_B} v_l^B + 1}$. To match this to the structure of $\phi_{\text{MIX}}(j, S_B)$, the MNL component's weight in our model, $\sum_{\ell \in \mathbf{N}_B \setminus S_B} \lambda_\ell$, would need to correspond to the fixed parameter $1 - \tilde{\lambda}$. However, since our model's weight term depends on the offered assortment S_B, it cannot be equated with a fixed parameter $1 - \tilde{\lambda}$.

Conversely, the mixed model cannot be represented by our model. To map ϕ_{MIX} to our model's structure, we would need to find a fixed set of parameters $(\lambda_j)_{j\in\mathbf{N}_B}$ for our model that reproduces the mixture models' probabilities for all products and assortments. This would require satisfying two conditions simultaneously: $\lambda_j = \tilde{\lambda}\tilde{\theta}_j$ and $1 - \sum_{j\in\mathbf{N}_B\setminus S_B}\lambda_j = 1-\tilde{\lambda}$ for all $j\in S_B$, $S_B\subseteq\mathbf{N}_B$. The second condition cannot hold for a fixed set of (λ_j) parameters as the assortment S_B changes. This fundamental inconsistency demonstrates that the two models are structurally distinct.

Appendix B: Omitted Details and Proofs in Section 3

B.1. Existence of Non-invariant Optimal Assortments for MC

EXAMPLE 1 (NON-INVARIANT OPTIMAL ASSORTMENTS). Not all optimal assortments for an MC model are invariant across different arrival distributions. Consider a category with two products $\{1,2\}$. Let 0 denote the outside option. The transition probabilities are $\rho_{1,0}=\rho_{2,0}=1$, and the revenues are $r_1=r_2=1$.

If the arrival probabilities $\psi_1=1,\ \psi_2=0$, an optimal assortment is $S^*=\{1\}$. However, if the arrival vector switches to $\psi_1=0,\ \psi_2=1$, then $\{1\}$ is no longer optimal; instead, either $S^*=\{2\}$ or $S^*=\{1,2\}$ is optimal.

This shows that some optimal assortments depend on the arrival distribution. Nevertheless, the maximal assortment $S^*=\{1,2\}$ is optimal for both arrival vectors, and hence serves as an invariant optimal assortment for this transition matrix $\boldsymbol{\rho}$.

B.2. Existence of Invariant Unconstrained Optimal Assortment under MC Model

LEMMA 10. *Let ϕ be a Markov chain choice model with price vector $\mathbf{r}$, transition matrix $\boldsymbol{\rho}$, and initial arrival probabilities $\boldsymbol{\psi}$. Then there exists an optimal unconstrained assortment under ϕ that depends only on $(\mathbf{r},\boldsymbol{\rho})$, and is independent of $\boldsymbol{\psi}$.*

Proof of Lemma 10. Blanchet et al. (2016) show that the optimal revenue-maximizing assortment for a Markov chain choice model can be found by solving a linear program (See Theorem 5.1 and Lemma 5.2 in Blanchet et al. (2016)). The constraints and objective function of this LP are constructed using only the price vector $\mathbf{r}$ and the transition matrix $\boldsymbol{\rho}$. Since the initial arrival probabilities $\boldsymbol{\psi}$ do not appear as parameters in this LP formulation, the solution, and thus the optimal assortment derived from it, is independent of $\boldsymbol{\psi}$.

Moreover, the iterative algorithm given by Désir et al. (2020) also yields an optimal assortment that is independent of the initial arrival probabilities, see Algorithm 1 and Theorem 2 in Désir et al. (2020). $\square$

B.3. Equivalence of Assortment Problems with a Non-Zero Price Outside Option

In this section, we show that an unconstrained assortment optimization problem where the outside option has a non-zero price can be transformed into an equivalent problem where the outside option has zero price. This allows standard assortment optimization algorithms, which often assumes a zero-price outside option, to be applied directly.

Let $\phi(i,S)$ be the probability of choosing product i from S^+. Let $(r_i)_{i\in\mathbf{N}^+}$ be a set of prices, where the price of the outside option, r_0, may be positive. The objective is to find the assortment $S^*\subseteq\mathbf{N}$ that solves:

$$\max_{S\subseteq\mathbf{N}} R(S) = \sum_{i\in S^+} r_i\cdot\phi(i,S). \tag{7}$$

LEMMA 11. *The optimal assortment S^* for the problem* (7) *is identical to the optimal assortment for the following problem with 'shifted' prices $r_i' = r_i - r_0$ for all $i \in \mathbf{N}^+$:*

$$\max_{S \subseteq \mathbf{N}} R'(S) = \sum_{i \in S^+} r_i' \cdot \phi(i, S). \tag{8}$$

Proof of Lemma 11. Let $c = r_0$ be the price of the outside option in the original problem. The shifted prices are defined as $r_i' = r_i - c$ for all $i \in \mathbf{N}^+$. Note that for the outside option, the shifted price is $r_0' = r_0 - c = r_0 - r_0 = 0$.

We can rewrite the original objective as:

$$\begin{aligned} R(S) &= \sum_{i \in S^+} r_i \cdot \phi(i, S) \\ &= \sum_{i \in S^+} (r_i' + c) \cdot \phi(i, S) \\ &= \sum_{i \in S^+} r_i' \cdot \phi(i, S) + \sum_{i \in S^+} c \cdot \phi(i, S) \\ &= R'(S) + c \sum_{i \in S^+} \phi(i, S) \end{aligned}$$

Since $\phi(\cdot, S)$ is a probability distribution over all possible options, the sum of probabilities is equal to one: $\sum_{i \in S^+} \phi(i, S) = 1$. Thus $R'(S)$ and $R'(S)$ differ only by the constant c for any S, which is independent of the assortment S. Hence, both problems have the same optimal solution S^*.

The problem (8) is a standard assortment optimization problem where the outside option has zero price. The only difference is that now the products could have negative prices. For any substitution-based choice model, products with negative prices can be ignored without loss of generality. Therefore, problem (8) can be solved by existing algorithms. □

B.4. Algorithms for DAG

We first present the algorithm for a general DAG.

Algorithm 2: Unconstrained Assortment Optimization in a General DAG

Input: A DAG $G = (\mathcal{V}, \mathcal{E})$, prices $r_{i_U}^U$ for products $i_U \in \mathbf{N}_U$, and choice models ϕ_U for each category $U \in \mathcal{V}$;

Let $(U_1, U_2, \ldots, U_{|V|})$ be a reverse topological ordering of the categories in $\mathcal{V}$;

for $n \leftarrow 1$ **to** $|V|$ **do**

  Let $U \leftarrow U_n$ be the current category;

  Define adjusted prices $(r_{i_U}')_{i_U \in \mathbf{N}_U}$ for products in U as:

$$r_{i_U}' \leftarrow r_{i_U}^U + \sum_{W \in \text{Children}(U)} \Big(\sum_{i_W \in S_W^{*,+}} \phi_{W|i_U}(i_W, S_W^*) r_{i_W}' \Big);$$

  Compute the optimal invariant unconstrained assortment S_U^* for U under ϕ_U using the adjusted prices $(r_{i_U}')_{i_U \in \mathbf{N}_U^+}$;

Return: The set of optimal assortments $\{S_U^*\}_{U \in \mathcal{V}}$.

To illustrate, consider a three-category chain $A \to B \to C$. The procedure begins at the terminal category C, where S_C^* is computed using its original prices (so $r_{i_C}' = r_{i_C}^C$). It then moves to category B. The adjusted price for each product i_B equals its original price plus the expected revenue from the fixed optimal assortment S_C^*, conditional on choosing i_B:

$$r'_{i_B} = r^B_{i_B} + \sum_{i_C \in S_C^*} \phi_{C|i_B}(i_C, S_C^*)\, r^C_{i_C}.$$

The optimal assortment S_B^* is then computed using these forward-looking prices. Finally, at category A, each product's adjusted price incorporates both its intrinsic price and the expected value of the entire $B \to C$ path, computed from the adjusted prices r'_{i_B}.

THEOREM 5. *For any DAG $G = (\mathcal{V}, \mathcal{E})$, Algorithm 2 computes an optimal set of assortments $\{S_U^*\}_{U \in \mathcal{V}}$ in polynomial time, provided the choice model ϕ_U of every category $U \in \mathcal{V}$ is a Markov chain choice model.*

The proof follows by backward induction, using the same decoupling argument as in the two-category case.

Proof of Theorem 5. The proof proceeds by backward induction on the nodes of the DAG, processed in a reverse topological order. We show that the algorithm correctly computes the optimal assortment for each category by solving a single-category assortment problem with adjusted prices that incorporate the maximum potential downstream revenue.

(i) **Base Case.** Consider any terminal category U in the DAG, for which the set of Children(U) is empty. The algorithm's adjusted price calculation for a product $i_U \in \mathbf{N}_U$ simplifies to $r'_{i_U} = r^U_{i_U}$, as the sum over an empty set is zero. The algorithm then computes the optimal assortment S_U^* using these prices. This is correct by definition, since the optimal unconstrained assortment for the MC model does not depend on the initial attraction probabilities.

(ii) **Inductive Hypothesis.** Assume that for a given category U, the algorithm has already correctly computed the optimal assortments S_W^* and adjusted prices r'_{i_W} for all descendant categoreis, and that r'_{i_W} represents the maximum expected total revenue from the subgraph rooted at the choice of product i_W.

(iii) **Inductive Step.** We show that the algorithm correctly computes the optimal assortment S_U^* for category U. The algorithm defines the adjusted price for a product $i_U \in \mathbf{N}_U$ as

$$r'_{i_U} \leftarrow r^U_{i_U} + \sum_{W \in \text{Children}(U)} \Big(\sum_{i_W \in S_W^{*,+}} \phi_{W|i_U}(i_W, S_W^*) r'_{i_W} \Big).$$

The second term on the right-hand side is the expected revenue from all downstream branches, conditional on choosing i_U. This calculation is valid due to two properties. First, the optimal unconstrained assortment S_W^* for the MC choice model ϕ_W is invariant to the initial attraction probabilities $\boldsymbol{\lambda}_W^{i_U}$, and thus does not depend on which i_U is chosen. This allows the use of the pre-computed S_W^*. Second, by the inductive hypothesis, the prices r'_{i_W} used in the calculation are the correct maximum revenues for the subproblems rooted at the choices i_W.

Therefore, r'_{i_U} correctly represents the total value of choosing product i_U, i.e., its Bellman value. By solving the single-category assortment problem for category U with these correctly specified adjusted prices, the algorithm finds the optimal assortment S_U^*.

By backward induction, the algorithm correctly computes the optimal assortment for all categories in the DAG. Thus, the returned set $\{S_U^*\}_{U \in \mathcal{V}}$ is globally optimal. □

B.5. Proof of Theorem 3.

To show the inapproximability, we perform a reduction from the Bipartite Densest κ-subgraph (BDκS) problem. We first define the problem and state the known hardness result from Chen et al. (2022).

DEFINITION 1. Given an undirected bipartite graph $G = (\mathbf{N}, \mathbf{M}, \mathbf{E})$ with vertex sets $\mathbf{N}$ and $\mathbf{M}$ and edge set $\mathbf{E} \subseteq \mathbf{N} \times \mathbf{M}$, the BD$\kappa$S problem is to find subsets $\mathbf{N}_1 \subseteq \mathbf{N}$ and $\mathbf{M}_1 \subseteq \mathbf{M}$ that solve:

$$\begin{aligned}&\max_{\mathbf{N}_1,\mathbf{M}_1} |E(\mathbf{N}_1 \times \mathbf{M}_1)|\\ &\text{s.t.} |\mathbf{N}_1| = |\mathbf{M}_1| = \kappa\,, \mathbf{N}_1 \subseteq \mathbf{N}\,, \mathbf{M}_1 \subseteq \mathbf{M},\end{aligned}$$

where $E(\mathbf{N}_1 \times \mathbf{M}_1)$ is the set of edges with one endpoint in $\mathbf{N}_1$ and the other in $\mathbf{M}_1$.

LEMMA 12 **(Lemma 6 in Chen et al. (2022))**. *There is a constant $c > 0$ such that, assuming Exponential Time Hypothesis (ETH), there is no $\Omega(g^{-1/(\log\log g)^c})$-approximation algorithm for BDκS defined on a bipartite graph with g vertices.*

Next, we prove the hardness of our cardinality-constrained problem.

Proof of Theorem 3. We now show that an efficient approximation algorithm for our cardinality-constrained assortment problem would imply an efficient approximation for BDκS. Consider an arbitrary bipartite graph $G = (\mathbf{N}_A, \mathbf{N}_B, \mathbf{E})$ and cardinality κ. Let $m = |\mathbf{N}_A| + |\mathbf{N}_B|$. We consider our two-category model with ϕ_A and ϕ_B as the MNL model. Let $r_i^A = 0$, $v_i^A = \frac{1}{m}$ for all $i \in \mathbf{N}_A$; $r_j^B = 1$, $v_j^B = 0$ for all $j \in \mathbf{N}_B$, and $\lambda_{i,j} = \frac{1}{m}\mathbb{1}_{(i,j)\in\mathbf{E}}$, $\lambda_{i,0} = 1 - \sum_{j\in\mathbf{N}_B} \frac{1}{m}\mathbb{1}_{(i,j)\in\mathbf{E}} > 0$. Let $K_A = K_B = \kappa$. Let $R(S_A, S_B)$ denote the expected revenue given assortments S_A and S_B. Then the cardinality-constrained problem is simplified as follows:

$$\max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} R(S_A,S_B) = \max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} \frac{\sum\limits_{i\in S_A}\sum\limits_{j\in S_B} \mathbb{1}_{(i,j)\in\mathbf{E}}\dfrac{1}{m^2}}{\sum\limits_{i\in S_A}\dfrac{1}{m}+1} \ge \max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} \frac{1}{2m^2}|E(S_A\times S_B)|. \tag{9}$$

Moreover, we have

$$\max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} R(S_A,S_B) = \max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} \frac{\sum\limits_{i\in S_A}\sum\limits_{j\in S_B} \mathbb{1}_{(i,j)\in\mathbf{E}}\dfrac{1}{m^2}}{\sum\limits_{i\in S_A}\dfrac{1}{m}+1} \le \max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} \frac{1}{m^2}|E(S_A\times S_B)|. \tag{10}$$

Suppose we can obtain a constant-factor approximation for the assortment problem, i.e., we have $\tilde{S}_A$, $\tilde{S}_B$ such that $R(\tilde{S}_A, \tilde{S}_B) \ge \alpha \max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} R(S_A, S_B)$ for a constant α, then we have:

$$\begin{aligned}|E(\tilde{S}_A\times\tilde{S}_B)| &\ge m^2\frac{\sum\limits_{i\in \tilde{S}_A}\sum\limits_{j\in \tilde{S}_B} \mathbb{1}_{(i,j)\in\mathbf{E}}\dfrac{1}{m^2}}{\sum\limits_{i\in \tilde{S}_A}\dfrac{1}{m}+1} = m^2R(\tilde{S}_A,\tilde{S}_B)\\ &\ge \alpha m^2 \max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} R(S_A,S_B) \ge \frac{\alpha}{2}\max_{\substack{S_A\subseteq\mathbf{N}_A,\,|S_A|\le\kappa\\ S_B\subseteq\mathbf{N}_B,\,|S_B|\le\kappa}} |E(S_A\times S_B)|.\end{aligned}$$

Here the first inequality is from the definition of $|E(\cdot)|$ and the last inequality is from inequality (9). Moreover, for any feasible solution (S_A, S_B) of the cardinality-constrained assortment problem, we can construct a (S'_A, S'_B) such that

$S_A \subseteq S'_A$, $S_B \subseteq S'_B$, $|S'_A| = |S'_B| = \kappa$, and $|E(S'_A \times S'_B)| \geq |E(S_A \times S_B)|$. Therefore, if $|\tilde{S}_A| < \kappa$ or $|\tilde{S}_B| < \kappa$, we can construct $\tilde{S}'_A$ and $\tilde{S}'_B$ such that $|\tilde{S}'_A| = |\tilde{S}'_B| = \kappa$ and $|E(\tilde{S}'_A \times \tilde{S}'_B)| \geq |E(\tilde{S}_A \times \tilde{S}_B)| \geq \frac{\alpha}{2} \max_{\substack{S_A \subseteq \mathbf{N}_A,\, |S_A| \leq \kappa \\ S_B \subseteq \mathbf{N}_B,\, |S_B| \leq \kappa}} |E(S_A \times S_B)|$, which yields a $\frac{\alpha}{2}$-approximation for the BDκS problem.

Appendix C: Omitted Details in Section 4

C.1. Example of Non-Concavity of the Log-Likelihood

The observed-data log-likelihood function in Equation (6) is generally not concave. We show this using a simple example. Consider a ground set $\mathbf{N}_A = \{i\}$ and $\mathbf{N}_B = \{j, m\}$. Suppose the purchase history $\mathcal{H}$ consists of a single observation: at time $t = 1$, the offered assortments were $S_A^1 = \{i\}$ and $S_B^1 = \{j\}$, and the customer purchased i and j. Then the log-likelihood function is $\log L(\boldsymbol{\lambda}, \mathbf{v}^A, \mathbf{v}^B; \mathcal{H}) = \log \frac{v_i^A}{v_i^A + 1} + \log\left(\lambda_{i,j} + \lambda_{i,m} \frac{v_j^B}{v_j^B + 1}\right)$. Replacing v_i^A with $\exp(\mu_i)$, the first term is concave in $\boldsymbol{\mu}$ and independent of the second term. Thus, the overall function is concave if and only if the second term is concave. Define

$$f(\mathbf{v}^B, \boldsymbol{\lambda}) = \log\left(\lambda_{i,j} + \lambda_{i,m} \frac{v_j^B}{v_j^B + 1}\right).$$

For simplicity, we omit the subscript i, writing $f(v_B, \boldsymbol{\lambda}) = \log\left(\lambda_j + \lambda_m \frac{v_j}{v_j + 1}\right)$. The following example shows that f is not concave in $(\lambda_j, \lambda_m, v_j^B)$.

Let the two parameter points be $\boldsymbol{\theta}_1 = (0.2611, 0.5875, 7.5261)$ and $\boldsymbol{\theta}_2 = (0.6689, 0.0783, 2.4141)$. Evaluating,

$$f(\boldsymbol{\theta}_1) = \log\left(0.2611 + 0.5875 \cdot \frac{7.5261}{7.5261 + 1}\right) = -0.2488,$$
$$f(\boldsymbol{\theta}_2) = \log\left(0.6689 + 0.0783 \cdot \frac{2.4141}{2.4141 + 1}\right) = -0.3225.$$

The average is $\frac{1}{2}(f(\boldsymbol{\theta}_1) + f(\boldsymbol{\theta}_2)) = -0.2857$. Now consider the midpoint $\boldsymbol{\theta}' = \frac{1}{2}(\boldsymbol{\theta}_1 + \boldsymbol{\theta}_2) = (0.4650, 0.3329, 4.9701)$, for which

$$f(\boldsymbol{\theta}') = \log\left(0.4650 + 0.3329 \cdot \frac{4.9701}{4.9701 + 1}\right) = -0.2982.$$

Since $f(\boldsymbol{\theta}') = -0.2982 < -0.2857 = \frac{1}{2}(f(\boldsymbol{\theta}_1) + f(\boldsymbol{\theta}_2))$, the function is not concave in $(\lambda_j, \lambda_m, v_j^B)$. This demonstrates that the observed-data log-likelihood is not, in general, a concave function of the model parameters.

C.2. EM Algorithm Details

E-step: computing $\hat{X}$. In the expectation step, we compute

$$\hat{X}_m^{t(l)} := \mathbb{E}[X_m^t \mid \mathcal{H}, \Theta^{(l)}] = P(X_m^t = 1 \mid a^t, b^t, S_A^t, S_B^t, \boldsymbol{\lambda}^{(l)}, \mathbf{v}^{B,(l)})$$

for all $m \in \mathbf{N}_B^+$ and $t \in [T]$. This probability can be written as

$$\hat{X}_m^{t(l)} = \frac{P(X_m^t = 1, b^t \mid a^t, S_A^t, S_B^t, \boldsymbol{\lambda}^{(l)}, \mathbf{v}^{B,(l)})}{P(b^t \mid a^t, S_A^t, S_B^t, \boldsymbol{\lambda}^{(l)}, \mathbf{v}^{B,(l)})}.$$

From Lemma 1, the denominator is

$$P(b^t \mid a^t, S_A^t, S_B^t, \boldsymbol{\lambda}^{(l)}, \mathbf{v}^{B,(l)}) = \lambda_{a^t, b^t}^{(l)} + \frac{v_{b^t}^{B,(l)}}{\sum_{k \in S_B^t} v_k^{B,(l)} + 1} \sum_{m \in \mathbf{N}_B \setminus S_B^t} \lambda_{a^t, m}^{(l)}.$$

The numerator can be understood in two cases. When $m = b^t$, the customer arrives at m and chooses m with probability $\lambda^{(l)}_{a^t,m}$. When $m \neq b^t$ and $m \notin S^t_B$, the customer first arrives at m and then jumps to b^t with probability $\frac{v^{B,(l)}_{b^t}}{\sum_{k\in S^t_B} v^{B,(l)}_k+1}$. Combining these, we obtain

$$\hat{X}^{t(l)}_m = \frac{\lambda^{(l)}_{a^t,m}\left(\mathbb{1}\{b^t = m\} + \mathbb{1}\{m \notin S^t_B\}\frac{v^{B,(l)}_{b^t}}{\sum_{k\in S^t_B} v^{B,(l)}_k+1}\right)}{\lambda^{(l)}_{a^t,b^t} + \frac{v^{B,(l)}_{b^t}}{\sum_{k\in S^t_B} v^{B,(l)}_k+1}\sum_{m\in \mathbf{N}_B\setminus S^t_B}\lambda^{(l)}_{a^t,m}}. \tag{11}$$

M-step: maximization. In the maximization step, we solve

$$\max_{(\mathbf{v}^A,\boldsymbol{\lambda},\mathbf{v}^B)\in\mathcal{P}} \log L_C(\Theta;\mathcal{H},\mathbf{X}),$$

where the complete-data log-likelihood decomposes as

$$\log L_C(\Theta;\mathcal{H},\mathbf{X}) = L_1(\mathbf{v}^A;\mathcal{H},\mathbf{X}) + L_2(\boldsymbol{\lambda};\mathcal{H},\mathbf{X}) + L_3(\mathbf{v}^B;\mathcal{H},\mathbf{X}),$$

with

$$L_1(\mathbf{v}^A;\mathcal{H},\mathbf{X}) = \sum_{t=1}^T \log\left(\frac{v^A_{a^t}}{V(S^t_A)+1}\right),$$

$$L_2(\boldsymbol{\lambda};\mathcal{H},\mathbf{X}) = \sum_{t=1}^T\sum_{m\in\mathbf{N}^+_B} X^t_m \log\lambda_{a^t,m},$$

$$L_3(\mathbf{v}^B;\mathcal{H},\mathbf{X}) = \sum_{t=1}^T\sum_{m\in\mathbf{N}^+_B} X^t_m \log\left(\mathbb{1}\{m=b^t\} + \mathbb{1}\{m\in\mathbf{N}_B\setminus S^t_B\}\frac{v^B_{b^t}}{V^B(S^t_B)+1}\right).$$

These three terms can be maximized separately. Since $\log x$ is concave in x, L_2 is concave in $\boldsymbol{\lambda}$. Moreover, L_1 is concave in $\boldsymbol{\alpha} = (\alpha_i)_{i\in\mathbf{N}_A}$ under the reparameterization $v^A_i = e^{\alpha_i}$, and L_3 is concave in $\mathbf{v}^B$ under the same reparameterization. Thus, each subproblem is concave in its respective parameters and can be solved efficiently using standard convex optimization methods.

C.3. Proof of Theorem 4

Proof of Theorem 4. The log-likelihood $L(\boldsymbol{\lambda},\mathbf{v}^A,\mathbf{v}^B)$ is continuous and differentiable in $(\boldsymbol{\lambda},\mathbf{v}^A,\mathbf{v}^B)$ over $\mathcal{P}$. In the E-step, the quantities $\hat{X}^t_b$ are continuous functions of $(\boldsymbol{\lambda},\mathbf{v}^A,\mathbf{v}^B)$, which implies that the complete-data log-likelihood L_C is also continuous in $(\hat{X}^t_b,\boldsymbol{\lambda},\mathbf{v})$. By Theorem 2 and Corollary 1 in Nettleton (1999), $L(\Theta^{(l+1)}) \geq L(\Theta^{(l)})$, for all $l \geq 1$, and $\{L(\Theta^{(l)})\}$ converges monotonically to $L(\Theta^*)$ for some stationary point Θ^*. $\square$

C.4. General DAG Estimation

Our estimation extends beyond the two-category MNL model. First, the choice model for the initial category, ϕ_A, can be any choice model with a known estimation routine. For a problem defined on a DAG, we introduce a set of latent variables for the initial attraction probabilities corresponding to each edge in the graph. The M-step of the EM algorithm then conveniently decomposes, allowing us to solve for the parameters of the choice model within each category and the transition probabilities $\boldsymbol{\lambda}$ for each edge separately.

The estimation framework is generalized to a model defined on a DAG $\mathcal{G} = (\mathcal{V},\mathcal{E})$, where $\mathcal{V}$ is the set of categories and $\mathcal{E}$ is the set of directed edges representing feasible transitions. The full parameter set is $\Theta =$

$(\{\mathbf{v}^U\}_{U\in\mathcal{V}}, \{\boldsymbol{\lambda}^{U,U'}\}_{(U,U')\in\mathcal{E}})$, where $\mathbf{v}^U$ are the parameters for the internal choice model ϕ_U of category U, and $\boldsymbol{\lambda}^{U,U'}$ is the matrix of transition probabilities for the edge (U,U'). The observed data $\mathcal{H}$ consists of transactions, each comprising a sequence of choices along a path in the DAG.

The core of the Expectation-Maximization (EM) algorithm is the introduction of latent variables to represent the unobserved initial interests of the customer. For each transaction t and each edge $(U,U')\in\mathcal{E}$, we define a latent variable $X_{i,m}^{t,(U,U')}$ to be 1 if the customer, after choosing product $i\in\mathbf{N}_U^+$, initially directs their attention to product $m\in\mathbf{N}_{U'}^+$, and 0 otherwise. Let $\mathbf{X}$ be the collection of all such latent variables. The complete-data log-likelihood $\log L_C(\Theta;\mathcal{H},\mathbf{X})$ can be formulated by conditioning on these latent events.

The key property of this formulation is that the complete-data log-likelihood decomposes into a sum of terms, each corresponding to a specific component of the model. This allows the objective function for the M-step, $Q(\Theta|\Theta^{(l)}) = \mathbb{E}_{\mathbf{X}|\mathcal{H},\Theta^{(l)}}[\log L_C(\Theta;\mathcal{H},\mathbf{X})]$, separates as:

$$Q(\Theta|\Theta^{(l)}) = \sum_{U\in\mathcal{V}} Q_U(\mathbf{v}^U|\Theta^{(l)}) + \sum_{(U,U')\in\mathcal{E}} Q_{U,U'}(\boldsymbol{\lambda}^{U,U'}|\Theta^{(l)}).$$

where each component function depends only on the parameters of a single category or a single transition edge.

The E-step at iteration ℓ involves computing the conditional expectation of each latent variable, $\hat{X}_{i,m}^{t,(U,U')(l)} = \mathbb{E}[X_{i,m}^{t,(U,U')}|\mathcal{H},\Theta^{(l)}]$. This posterior probability is calculated using Bayes' rule based on the observed choices in the transaction path and the current parameter estimates $\Theta^{(l)}$.

The M-step leverages the decomposition of $Q(\Theta|\Theta^{(l)})$ to update the parameters by solving a set of independent maximization problems. For each category $U\in\mathcal{V}$, the parameter update for the within-category choice model is given by:

$$\mathbf{v}^{U,(l+1)} = \arg\max_{\mathbf{v}^U} Q_U(\mathbf{v}^U|\Theta^{(l)}).$$

This subproblem is equivalent to a weighted maximum likelihood estimation for the choice model ϕ_U, where the weights are derived from the expected latent variables computed in the E-step. For each edge $(U,U')\in\mathcal{E}$, the update for the transition probabilities has a closed-form solution. The objective $Q_{U,U'}(\boldsymbol{\lambda}^{U,U'}|\Theta^{(l)})$ is a sum of weighted logarithms of the transition probabilities, $\sum_{t\in[T]}\sum_{i\in\mathbf{N}_A^+}\sum_{m\in\mathbf{N}_B^+}\hat{X}_{i,m}^{t,(U,U')(l)}\log\lambda_{i,m}^{U,U'}$. Maximizing this subject to $\sum_{m\in\mathbf{N}_{U'}^+}\lambda_{i,m}^{U,U'}=1$ for each $i\in\mathbf{N}_U^+$ yields the intuitive update rule:

$$\lambda_{i,m}^{U,U',(l+1)} = \frac{\sum_{t=1}^T \hat{X}_{i,m}^{t,(U,U')(l)}}{\sum_{t=1}^T\sum_{m'\in\mathbf{N}_{U'}^+}\hat{X}_{i,m'}^{t,(U,U')(l)}}.$$

This corresponds to normalizing the expected number of transitions from product i to product m.

Appendix D: Additional Experiment Results

D.1. Tables for Synthetic Data Results

D.1.1. Model Fit and Prediction Accuracy See Table 4, 5 and 6.

D.1.2. Revenue Lift See Table 7, 8 and Figure 9.

Table 4 Log-likelihood results on synthetic data for varying values of θ. Values in parentheses indicate the percentage improvement relative to INDMNL.

θ	Train Log-Likelihood			Test Log-Likelihood		
	INDMNL	MARKOVMNL	MULTIMNL	INDMNL	MARKOVMNL	MULTIMNL
0.0	-9103.84	-8587.60 (+5.67%)	-9066.26 (+0.41%)	-3857.57	-3661.53 (+5.08%)	-3899.41 (−1.08%)
0.5	-9203.67	-8695.58 (+5.52%)	-9081.49 (+1.33%)	-3942.27	-3751.33 (+4.84%)	-3959.21 (−0.43%)
1.0	-9635.82	-9091.37 (+5.65%)	-9359.05 (+2.87%)	-4141.34	-3947.13 (+4.69%)	-4073.74 (+1.63%)
1.5	-10235.34	-9528.98 (+6.90%)	-9761.74 (+4.63%)	-4389.02	-4118.61 (+6.16%)	-4234.36 (+3.52%)
2.0	-10668.46	-9950.38 (+6.73%)	-10139.78 (+4.96%)	-4599.91	-4319.16 (+6.10%)	-4436.37 (+3.56%)
2.5	-10725.67	-9917.84 (+7.53%)	-10088.72 (+5.94%)	-4591.35	-4270.19 (+6.99%)	-4378.37 (+4.64%)
3.0	-10783.88	-9936.01 (+7.86%)	-10125.77 (+6.10%)	-4627.33	-4288.25 (+7.33%)	-4414.15 (+4.61%)
3.5	-11083.00	-10263.56 (+7.39%)	-10434.62 (+5.85%)	-4765.41	-4426.32 (+7.12%)	-4545.45 (+4.62%)
4.0	-11050.78	-10208.97 (+7.62%)	-10354.45 (+6.30%)	-4743.70	-4405.65 (+7.13%)	-4493.68 (+5.27%)
4.5	-11180.35	-10324.91 (+7.65%)	-10490.16 (+6.17%)	-4799.32	-4467.11 (+6.92%)	-4559.96 (+4.99%)
5.0	-11476.66	-10523.26 (+8.31%)	-10702.31 (+6.75%)	-4930.02	-4547.18 (+7.77%)	-4643.27 (+5.82%)

Table 5 Top-3 hit rate (test set) for synthetic data. Values in parentheses represent the difference in percentage points (p.p.) relative to INDMNL.

θ	INDMNL	MARKOVMNL	MULTIMNL
0.0	0.9520	0.9567 (+0.47 p.p.)	0.9487 (-0.33 p.p.)
0.5	0.9446	0.9526 (+0.80 p.p.)	0.9471 (+0.25 p.p.)
1.0	0.9247	0.9352 (+1.05 p.p.)	0.9323 (+0.76 p.p.)
1.5	0.8977	0.9217 (+2.40 p.p.)	0.9154 (+1.77 p.p.)
2.0	0.8860	0.9096 (+2.36 p.p.)	0.9027 (+1.67 p.p.)
2.5	0.8863	0.9131 (+2.68 p.p.)	0.9105 (+2.42 p.p.)
3.0	0.8765	0.9110 (+3.45 p.p.)	0.9048 (+2.83 p.p.)
3.5	0.8662	0.8973 (+3.11 p.p.)	0.8929 (+2.67 p.p.)
4.0	0.8682	0.8980 (+2.98 p.p.)	0.8932 (+2.50 p.p.)
4.5	0.8658	0.8933 (+2.75 p.p.)	0.8874 (+2.16 p.p.)
5.0	0.8460	0.8877 (+4.17 p.p.)	0.8798 (+3.38 p.p.)

Table 6 Rank accuracy (test set) for synthetic data (lower is better). Values in parentheses represent the percentage increase relative to INDMNL.

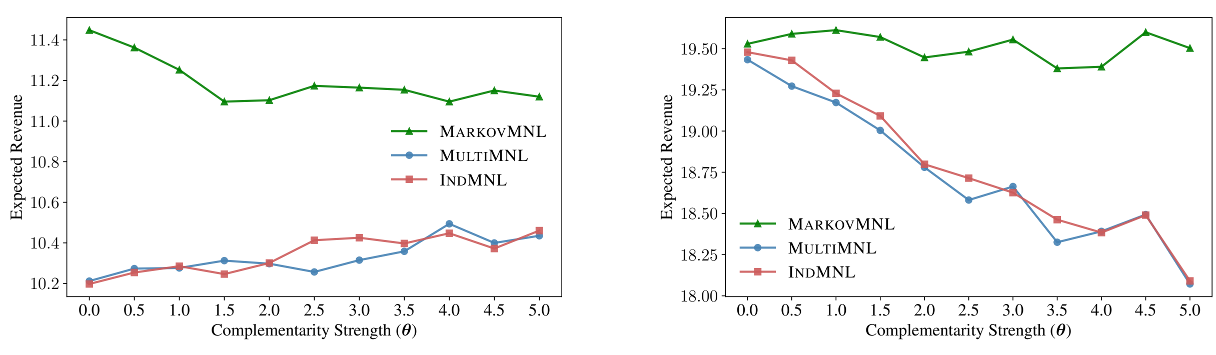
θ	INDMNL	MULTIMNL	MARKOVMNL
0.0	1.6907	1.6947 (+0.24%)	1.6579 (-1.94%)
0.5	1.7108	1.7010 (-0.57%)	1.6827 (-1.64%)
1.0	1.7800	1.7550 (-1.40%)	1.7339 (-2.59%)
1.5	1.9115	1.8471 (-3.37%)	1.8254 (-4.51%)
2.0	1.9964	1.9098 (-4.34%)	1.8862 (-5.53%)
2.5	1.9923	1.8893 (-5.16%)	1.8726 (-6.00%)
3.0	1.9975	1.8934 (-5.21%)	1.8718 (-6.31%)
3.5	2.0655	1.9427 (-5.94%)	1.9248 (-6.81%)
4.0	2.0595	1.9313 (-6.23%)	1.9172 (-6.91%)
4.5	2.0888	1.9642 (-5.98%)	1.9465 (-6.80%)
5.0	2.1433	2.0065 (-6.39%)	1.9797 (-7.64%)

Table 7 **Expected revenues for low price sensitive products. Values in parentheses indicate percentage change relative to INDMNL.**

	Uniform Price Distribution			Normal Price Distribution		
θ	INDMNL	MULTIMNL	MARKOVMNL	INDMNL	MULTIMNL	MARKOVMNL
0.0	10.20	10.21 (+0.10%)	11.45 (+12.25%)	123.15	123.16 (+0.01%)	145.79 (+18.38%)
0.5	10.25	10.27 (+0.20%)	11.36 (+10.83%)	123.48	122.40 (-0.87%)	145.15 (+17.55%)
1.0	10.29	10.28 (-0.10%)	11.25 (+9.33%)	125.40	124.67 (-0.58%)	143.40 (+14.35%)
1.5	10.25	10.31 (+0.59%)	11.10 (+8.29%)	125.93	126.29 (+0.29%)	141.46 (+12.33%)
2.0	10.30	10.30 (+0.00%)	11.10 (+7.77%)	125.51	124.21 (-1.04%)	141.34 (+12.61%)
2.5	10.41	10.26 (-1.44%)	11.17 (+7.30%)	127.70	124.38 (-2.60%)	142.60 (+11.67%)
3.0	10.43	10.32 (-1.05%)	11.16 (+7.00%)	127.59	125.35 (-1.76%)	140.59 (+10.19%)
3.5	10.40	10.36 (-0.38%)	11.15 (+7.21%)	126.38	125.78 (-0.47%)	142.87 (+13.05%)
4.0	10.45	10.49 (+0.38%)	11.10 (+6.22%)	128.26	129.92 (+1.29%)	143.03 (+11.52%)
4.5	10.37	10.40 (+0.29%)	11.15 (+7.52%)	127.44	128.00 (+0.44%)	141.56 (+11.08%)
5.0	10.46	10.44 (-0.19%)	11.12 (+6.31%)	129.24	129.16 (-0.06%)	142.46 (+10.23%)

Table 8 **Expected revenues for high price sensitive products. Values in parentheses indicate percentage change relative to INDMNL.**

	Uniform Price Distribution			Normal Price Distribution		
θ	INDMNL	MULTIMNL	MARKOVMNL	INDMNL	MULTIMNL	MARKOVMNL
0.0	19.48	19.53 (+0.26%)	19.43 (-0.26%)	134.53	134.73 (+0.15%)	134.35 (-0.13%)
0.5	19.43	19.59 (+0.82%)	19.27 (-0.82%)	134.20	135.18 (+0.73%)	133.59 (-0.45%)
1.0	19.23	19.61 (+1.98%)	19.17 (-0.31%)	132.46	135.31 (+2.15%)	132.07 (-0.29%)
1.5	19.09	19.57 (+2.51%)	19.00 (-0.47%)	131.35	134.87 (+2.68%)	131.91 (+0.43%)
2.0	18.80	19.45 (+3.46%)	18.78 (-0.11%)	128.93	135.11 (+4.79%)	128.89 (-0.03%)
2.5	18.71	19.48 (+4.12%)	18.58 (-0.67%)	128.10	134.67 (+5.13%)	127.57 (-0.41%)
3.0	18.63	19.56 (+5.00%)	18.66 (+0.16%)	127.25	134.67 (+5.83%)	127.35 (+0.08%)
3.5	18.46	19.38 (+4.98%)	18.33 (-0.71%)	125.64	133.37 (+6.15%)	124.59 (-0.84%)
4.0	18.38	19.39 (+5.49%)	18.39 (+0.05%)	125.52	133.99 (+6.75%)	126.26 (+0.59%)
4.5	18.49	19.60 (+6.00%)	18.49 (+0.00%)	126.50	135.08 (+6.77%)	127.14 (+0.51%)
5.0	18.09	19.50 (+7.79%)	18.07 (-0.11%)	122.70	134.61 (+9.72%)	123.27 (+0.47%)



(a) Low Price Sensitivity (Uniform Dist.) (b) High Price Sensitivity (Uniform Dist.)

Figure 9 **Comparison of expected revenue under the Uniform price distribution.**

D.2. Real-data Case Study: Extension to Three Product Groups

A key advantage of our framework is its ability to model and optimize assortments across more than two product groups. To demonstrate this, we extend the 'Meats and Buns' case study by introducing a third group (category C)

of relevant condiments, including cheese, pickles, and mayonnaise, etc. This creates a sequential choice model, $A \to B \to C$, where the condiment choice is conditioned on the bun chosen, which itself is conditioned on the meat. We acknowledge that other dependency structures, such as a tree $B \leftarrow A \to C$, but our goal here is to demonstrate the framework's ability to capture complex multi-stage dependencies, for which the chain structure provides a clear and powerful example. To evaluate performance in this setting, we adapt our metrics accordingly. The total log-likelihood is the sum for choices in B and C. Similarly, the overall rank accuracy is the sum of the ranks for the choices in B and C, and hit rates are measured for the (B, C) pair conditional on the choice in A.

The results are summarized in Table 9. The MARKOVMNL model demonstrates a clear advantage in model fit, improving the out-of-sample LL by 10.44% over INDMNL, which is nearly double the improvement of the MULTIMNL model. While both complementarity models offer similar gains in hit rates, this confirms that our MARKOVMNL model is capable of capturing these complex dependencies with superior overall fit.

Table 9 Model fit and prediction accuracy for three groups (meats → buns → condiments). For LL and Rank Acc., parenthetical values are relative improvements over INDMNL. For HR and EHR, they are absolute differences in percentage points (p.p.).

Model	In-Sample LL	Out-of-Sample LL	top-3 HR	EHR_3	Rank Acc.
INDEPMNL	-193735.82	-82943.01	62.26%	1.63%	7.24
MULTIMNL	-182030.43 (+6.04%)	-78308.17 (+5.59%)	64.93% (+2.67 p.p.)	2.39% (+0.76 p.p.)	6.14 (-15.19%)
MARKOVMNL	-172070.40 (+11.18%)	-74285.83 (+10.44%)	65.01% (+2.75 p.p.)	2.36% (+0.73 p.p.)	6.12 (-15.47%)