Multi-Purchase Behavior: Modeling and Optimization

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We study the problem of modeling purchase of multiple items and utilizing it to display optimized recommendations, which is a central problem for online e-commerce platforms. Rich personalized modeling of users and fast computation of optimal products to display given these models can lead to significantly higher revenues and simultaneously enhance the end user experience. We present a parsimonious multi-purchase family of choice models called the BundleMVL-K family, and develop a binary search based iterative strategy that efficiently computes optimized recommendations for this model. This is one of the first attempts at operationalizing multi-purchase class of choice models. We characterize structural properties of the optimal solution, which allow one to decide if a product is part of the optimal assortment in constant time, reducing the size of the instance that needs to be solved computationally. We also establish the hardness of computing optimal recommendation sets. We show one of the first quantitative links between modeling multiple purchase behavior and revenue gains. The efficacy of our modeling and optimization techniques compared to competing solutions is shown using several real world datasets on multiple metrics such as model fitness, expected revenue gains and run-time reductions. The benefit of taking multiple purchases into account is observed to be 6 – 8% in relative terms for the Ta Feng and UCI shopping datasets when compared to the MNL model for instances with ~ 1500 products. Additionally, across 8 real world datasets, the test log-likelihood fits of our models are on average 17% better in relative terms. The simplicity of our models and the iterative nature of our optimization technique allows practitioners meet stringent computational constraints while increasing their revenues in practical recommendation applications at scale, especially in e-commerce platforms and other marketplaces.

Key words: Multi-choice purchase behavior, recommendations, scalable algorithms, structural properties.
1. Introduction

In both online and offline shopping, consumers typically purchase multiple products. Multiple purchases can happen due to complementarity, neighborhood affects (i.e., due to certain items shown or placed next to each other), or due to overlap in the purchase frequencies of various products (sometimes across unrelated categories) (Manchanda et al. 1999). All these effects may not be active simultaneously, and difficult to measure directly. Further, given an expressive choice model that captures this behavior, it is a priori unclear how to optimize for the product recommendations that the platform should ideally show to consumers as these tend to be hard combinatorial optimization problems. The ability to capture a rich enough choice behavior of each consumer as well as to display real-time optimized recommendations to them can have a tremendous impact on the user experience and hence the bottom-line of online shopping platforms. Given that online shopping is one of the most popular activities on the Internet world wide, with sales projected to exceed 6.5+ trillion US dollars by 2022 (Clement 2019), such a personalization effort can yield significant dividends.

Addressing the above challenges, we consider a parsimonious family of multi-purchase choice models (i.e. models capturing purchase of more than one products in an interaction), called the bundle multivariate logit models (BundleMVL-K), which is inspired by multiple variations proposed in the marketing literature (Cox 1972, Russell and Petersen 2000, Hruschka et al. 1999, Singh et al. 2005). It models the conditional probability of purchasing a product given the purchase/no-purchase of all other products and parsimoniously extends the popular multinomial choice model (MNL) to the setting where the customer purchases one or more items (represented by the suffix $K \in \mathbb{Z}_+$ in the acronym) when they are shown a set of recommendations. While modeling multiple purchases has been addressed in the marketing literature, with the end goal of improving customer understanding, the application of BundleMVL-K to recommendation sets of products (not just categories) and subsequent optimization based on it with a focus on its use in web scale settings is new to this work. We contrast
BundleMVL-K to existing single-choice and multi-choice models (Benson et al. 2018), deliberate on the optimal choice of K based on practical considerations, and validate the model performance (in terms of likelihood) on eight real datasets. For instance, BundleMVL-K’s parameters allow for interpreting substitution behavior and complementary relationships between products. Model fit (assessed using out of sample log likelihood values) when compared against state of the art multi-choice models shows that the BundleMVL-2 (i.e., K = 2) is a strong candidate in capturing rich multi-choice behavior of customers. In particular, we show that the benefit of taking multiple purchases into account in terms of revenue and sales is at least 6 – 8% in relative terms when compared to the MNL (this is for 1500 products, for other revenue improvement comparisons see Section 5). In addition, across 8 real world datasets, the test log-likelihood fits of our multi-purchase model are on average 17% better. Our approach addresses the key future direction discussed in the practice paper by Feldman et al. (2019), who establish strong evidence of the utility of single choice models in a product display setting at the firm Alibaba.

This work is one of the first attempts focused on optimizing revenue for multi-purchase choice models, allowing us to make a link between the model and the revenue gains that it allows. Most prior work, especially in the marketing literature, has not be able to establish this this, understandably due to complexity of the revenue optimization problems involved. In particular, assuming that each customer has a distinct BundleMVL-K model associated with them, we develop an iterative binary search based optimization scheme for computing approximately revenue optimal recommendations, while balancing its computational time and solution quality. We complement this by deriving several structural results about the optimal solution that help efficiently explore the search space, as well as by establishing the hardness of the problem (showing that it is indeed NP-complete when K = 2, compared to linear time when K = 1). The structural results allow our algorithms to determine if a product is part of the optimal solution or not with certainty in constant time, which allows us to work with smaller problem instances computationally. The binary search based algorithm solves a quadratic unconstrained binary optimization problem in each comparison step (we show how to solve
this practically using state of the art heuristic approximation techniques as well). Our approach is compared against a mixed integer programming benchmark, a natural greedy approach that extends the Adxopt algorithm developed for the MNL single-choice model \cite{Jagabathula2014} and the revenue-ordered heuristic among others. We also shed light on the properties of the solutions obtained using these benchmarks and when they perform optimally. Our solution to the revenue optimal recommendation problem is one of the first that is also practical and scalable for this class of models. The operational value of our algorithms is that they allow practitioners to capture additional revenue by being able to compute near optimal highly relevant recommendations at scale, hence minimizing the impact on customer disengagement due to computational delays that is typically observed in online platforms \cite{Palmer2016}. Along the way, we also make progress on the theoretical and computational tractability of recommendation set optimization under another natural multi-choice model proposed in \cite{Benson2018}, and illustrate how the BundleMVL-K model and recommendations based on it provide superior performance. Our empirical results on multiple real world datasets strongly support the possibility of real-time personalization that captures rich multi-purchase choice behavior. Table 1 outlines the list of our results and algorithmic techniques.

Section 2 describes the BundleMVL-K family of choice models. In Section 3, we state the revenue optimization problem and derive structural properties of the optimal solution, which we use in developing an iterative binary search based approach (Section 4). Extensive numerical experiments are detailed in Section 5. A brief discussion in Section 6 is followed by a conclusion in Section 7. All proofs are delegated to the appendix. Key prior work related to the problem and our solution approach are discussed next.

| Results | Section |
|---------|---------|
| Model: BundleMVL-2 - Estimation (Lem. 1, Alg. 3) - Hardness (Thm. 4, and structural properties (Lem. 2)) - BinarySearchAO (Alg. 6, 9) - BinarySearchAO(Efficient)(Alg. 2) - NoisyBinarySearchAO(Efficient) - Integer program (Alg. 4, 5) - Revenue-ordered (Thm. 3, 4) | 2 & appendix 3 4 6 8 9 11 11.2 appendix appendix appendix 4.3 3.1 |
| Model: MMC - Hardness (Thm. 2) | 3.1 |

Table 1: Summary of results.

Figure 1: CDF of the number of products purchased per transaction in the Walmart dataset.
1.1. Relevant Literature

Though purchasing multiple products by customers is extremely common in both online platforms and brick and mortar stores, the majority of research in choice modeling has focused on single product purchases. Train (2009) gives a good overview of the commonly used choice models, which include the MNL model (Plackett 1975), the nested logit model and others. More recently, a variety of other choice models such as the Markov chain choice model, the distribution over ranking models have been proposed and studied. Most work here concerns with both the estimation of the model from data, as well as the design of algorithms for revenue maximizing choice sets (assortments) and other related objectives. Some works have pursued robust algorithms, such as the Adxopt (Jagabathula 2014), designed to be choice model agnostic, while others have tried to capture various business-driven constraints, such as a constraint on the number of products that can be recommended, precedence constraints among products etc. (Rusmevichientong et al. 2010a, Sinha and Tulabandhula 2020). We refer the readers to Kök et al. (2008) for an overview of these optimization methods. In many datasets, some of which are explored here, only a minority percentage of transactions reflect single purchases, supporting the need for multi-purchase modeling that better reflect reality.

In the marketing literature, multi-choice models have appeared in the context of modeling purchase of products in multiple categories (Seetharaman et al. 2005) as well as in bundle choice modeling. Two types of choice models have been predominant here - the multivariate probit (MVP) and variants of the multivariate logit (MVL). Both of these models are based on the random utility theory. The earliest variation of MVL was proposed in Cox (1972) and has been used and improved upon in various subsequent works such as Russell and Petersen (2000) and Singh et al. (2005). In bundle choice modeling (McCardle et al. 2007), consumer choice is modeled at the level of product bundles instead of the category of products. Both the MVL variants (Kopalle et al. 1999) and the MVP model have also been considered for this task. Recently, neural network based multi-choice models have also been proposed (Yang and Sudharshan 2019) to capture multi-purchase behavior. While they are able to fit observed data much better than the parametric models considered here, the resulting
recommendation set optimization problems become quickly intractable due to lack of structure. Even with parametric models (such as ours), the optimization problems tend to be NP-hard, and in this paper, we devote significant effort to tame this complexity to make recommendation set computations scalable. A distinct problem that parallels our work is that of bundle pricing and optimization, where instead of computing recommendation sets that take choice behavior into account, one models how to price groups of products to maximize sales and revenue, see Ettl et al. (2020) and references therein.

A key prior work is by Benson et al. (2018) who propose a MVL variant, which we refer to as the Mixture Multi-Choice (MMC) model. This model assumes that the mean utility of any subset of products is the sum of the utilities of each product in the subset and an optional correction term. By limiting the number of sets which receive a correction, this model can have a sparse parameterization. A crucial drawback of this model is that the random variables that affect the probability of choosing bundles with overlapping products are assumed independent.

Immorlica et al. (2018) consider a choice model based on vertical customer differentiation, i.e., the ordering of utility of products is unambiguous and is the same for all customers, but customers differ in how much value they extract from the products. Unlike them, we study a horizontally differentiated choice model, with different customers having different utility maximizing sets. While Immorlica et al. (2018) focus on hardness results for the corresponding optimization problem, we restrict ourselves to bundles of size at most two for much of the paper (specializing the BundleMVL-K model family), and focus on designing scalable practical algorithms with extensive benchmarks, so that they can be readily used for near real-time personalization on e-commerce platforms.

2. The BundleMVL Choice Model For Multi-Purchase Behavior

The family of multi-purchase choice models that we formulate and study in this work, namely the BundleMVL-K family, has roots in the Marketing and the Spatial Statistics literature (Russell and Petersen 2000). Models in this family describe the probability with which a customer purchases a bundle $S$ (with $|S| \leq K$) of unique products when the platform recommends set $C$ of products. Thus, the suffix $K$ parameterizes these models by the maximum size of bundles that a customer can purchase.
(for instance, BundleMVL-2 model captures purchases of bundles of size at most 2). We start by specifying the conditional utility (a conditional random variable) of purchasing a product given the purchase decisions corresponding to all other products that were offered for the generic BundleMVL-K model as:

\[
U(i|\{X_j = x_j : j \in C, j \neq i\}) = \left(\alpha_i + \sum_{j \in C, j \neq i} \beta_{ij} x_j + \epsilon_i\right) I\left\{\sum_{j \in C, j \neq i} x_j < K\right\},
\]

where \(\alpha_i\) is a product specific parameter, parameters \(\beta_{ij}\) capture interactions between product pairs \(i\) and \(j\), \(\epsilon_i\) is a noise random variable distributed according to the Gumbel distribution, \(I\{\}\) is the indicator function that evaluates to one (zero) if the inequality is true (false), and \(X_j\) represent binary random variables that signify whether the customer purchased item \(j\) or not (\(x_j\) are the corresponding realizations) when \(C\) is offered. The \(\beta_{ij}\) parameters are symmetric in the product pair, i.e., \(\beta_{ij} = \beta_{ji}\). We can interpret from the above equation that the conditional utility of adding a product to a purchased bundle depends on its intrinsic value and its pairwise relationship with other purchases. Thus, even if the bundles are of size \(K\), the effect on the utility by other products is pairwise, restricting the number of parameters to be of \(O(n^2)\), where \(n\) is the number of products.

If the consumer has made a decision for each of the other products, then they will purchase product \(i\) only if the above conditional utility exceeds the threshold value 0. The conditional probability of buying product \(i \in C\) can be computed as:

\[
P(X_i = 1|\{X_j = x_j : j \in C, j \neq i\}) = \frac{\exp(\alpha_i + \sum_{j \in C, j \neq i} \beta_{ij} x_j)}{\exp(\alpha_i + \sum_{j \in C, j \neq i} \beta_{ij} x_j) + 1} I\left\{\sum_{j \in C, j \neq i} x_j < K\right\}.
\]

Note that the above probability is non-zero only when the number of products already purchased is strictly less than \(K\). These conditional probabilities can be combined using Besag’s characterization theorem [Besag, 1974] to get a consistent joint probability distribution of purchase of bundles. Let \(\phi\) be the empty bundle signifying a no-purchase event. As per Besag’s theorem, for any \(x = (x_1, \cdots x_n)\) such that \(P(x) > 0\), we have \(\frac{P(x)}{P(\phi)} = \prod_{i \in C} \frac{g^i(x_i)}{g^i(0)}\), where \(g^i(1) + g^i(0) = 1\) and:

\[
g^i(1) = \frac{\exp(\alpha_i + \sum_{j \in C, j < i} \beta_{ij} x_j)}{\exp(\alpha_i + \sum_{j \in C, j < i} \beta_{ij} x_j) + 1} I\left\{\sum_{j \in C, j < i} x_j < K\right\}.
\]
Thus, \( \frac{P(x)}{P(\phi)} = \exp\left( \sum_{i \in C} \alpha_i + \sum_{i \in C} \sum_{j \in C, j < i} \beta_{ij} x_j \right) \) if \( \sum_{j \in C, j < i} x_j < K \) = 1 and 0 otherwise. Using the fact that the sum of probability of purchase over all bundles is one, we get the probability of purchase of a bundle \( S \) given \( C \) as: \( P(S) = \frac{V_S}{1 + \sum_{S' \subseteq C, |S'| \leq K} V_{S'}} \), where \( V_S = \exp\left( \sum_{i \in C} \alpha_i x_i + \sum_{i \in C} \sum_{j \in C, j < i} \beta_{ij} x_i x_j \right) \) for all \( S \subseteq C, |S| \leq K \), and \( x_j = 1 \) if \( j \in S \) and zero otherwise. This expression lends itself to a high degree of interpretability (positive \( \beta_{ij} \) implying complementary and the opposite substitution relations), and intuitively suggests that bundles with large positive values of the intrinsic parameters (\( \alpha_i \)s) and large positive pairwise affinity values (\( \beta_{ij} \)s) will have a higher probability of being purchased. Note that one can extend our model representation power by including parameters involving three or more products as well, because as long as we ensure that the conditional probability of purchasing an product does not depend on the order of previous purchases, Besag’s theorem can still be used to derive an analogous multi-purchase model. To be consistent with the literature on single-choice models, we introduce another parameter \( \nu_0 \) corresponding to the no-purchase probability by scaling each \( V_S \) by \( \frac{1}{\nu_0} V_S \). One can interpret this parameter as the result of comparing the conditional utilities to a non-zero threshold.

A key point to note is that the model is not derived based on assigning a mean utility to every bundle, adding a random noise term and deriving purchase probabilities based on the utility maximizing bundle. Instead, the model assumes a form on the conditional utility of purchase of a product given the purchase decision on all other products and derives the only joint distribution consistent with this conditional probability distribution.

While precursors to the BundleMVL-K family exist in the literature, our key contribution here is two fold: (a) we extend these precursors to the modeling of multiple products in addition to categories (a category is a collection of similar products), and (b) we are able to restrict the number of products purchased to a parameterized value \( K \), and still obtain the softmax (or sigmoidal) structure of the probability of purchase expression above. This restriction parametrized by \( K \) and the softmax structure are both very appealing from an optimization perspective (see Section 4). For instance, the MNL single-choice model also has a similar form, which allows for the expected revenue maximizing
set computation in polynomial time. We achieve these two properties without making a restrictive assumption that is made for many other random utility models in the literature (Benson et al. 2018): they assume independent Gumbel perturbations to the utilities of bundles, even if these bundles share products between them.

With increasing values of $K$, we can model customers that purchase larger bundles ($K = 1$ gives us the MNL model). The model parameterization $(\alpha, \beta)$ remains the same for $K \geq 2$, although the data likelihood changes. The choice of $K$ is driven by the suitability of the model to data, and the tractability of the optimization problems (maximizing expected revenue or probability of purchase) downstream. For example, if most customers buy less than say 10 products, although choosing $K$ as 10 in the BundleMVL-K model suffices (see Figure 1), it may still be prudent to trade-off model fit with the computational tractability of optimization (by choosing a smaller value of $K$). As we show in Section 5, the choice of $K = 2$ strikes a great balance for many real world datasets in terms of fit and in terms of scalability of personalization. In particular, we show that on one hand the revenue gains achieved by using the BundleMVL-2 model over the MNL model can be large especially as the number of products grow, and on the other hand optimizing over BundleMVL-2 is much more empirically tractable (more revenue gains in a small fraction of time) when compared to BundleMVL-3.

Any BundleMVL-K model can be estimated directly using maximum likelihood estimation (MLE). Let $\{S_i, C_i\}_{i=1}^m$ be the dataset that potentially includes no purchase observations and $\max|S_i| \leq K$. Then the likelihood of observing the given data is:

$$P_{data} = \prod_{i=1}^m P(S_i|C_i \text{ was offered}) = \prod_{i=1}^m \left( \frac{\exp \left( \sum_{i \in S_i} \alpha_i + \sum_{i,j \in S_i, i<j} \beta_{ij} \right)}{v_0 + \sum_{S' \subseteq C_i, |S'| \leq K} \exp \left( \sum_{i \in S'} \alpha_i + \sum_{i,j \in S', i<j} \beta_{ij} \right)} \right),$$

which can be maximized numerically using, say first order methods, to get estimates of $\alpha_i$s and $\beta_{ij}$s.

The estimation problem becomes easy when $K = 2$ because one can optimize directly over $V_S$.

**Lemma 1.** Given values $V_S$ for all bundles $S$ of size $\leq 2$, we can uniquely obtain the parameters $(\alpha, \beta)$ by solving the system of equations: $\log V_S = \sum_{i \in S} \alpha_i + \sum_{i,j \in S, j > i} \beta_{ij}$ for all $S$.

Further, if the data is such that the same recommendation set is show to consumers in each observation, then $V_S$ can be estimated by simply counting and normalizing, which is a linear time
computation. Because of the equivalence above, we will use $V_S$ as parameters in the rest of the paper when working with BundleMVL-2.

3. Revenue Maximization: Hardness and Structural Results

Maximizing revenue from a set of offered products is one of the key goals of online/offline retailers. Under the BundleMVL-K model, the expected revenue of the platform if it offers recommendations $C$ is given by

$$R_K(C) = \sum_{S \subseteq C, |S| \leq K} V_S r_S v_0 + \sum_{S \subseteq C, |S| \leq K} V_S r_S,$$

where $r_S = \sum_{i \in S} r_i$, and $r_i > 0$ is the fixed and known revenue corresponding to product $i \in W$ and $W = \{1, 2, \ldots, n\}$ is the set of all products. We assume that the products are ordered such that $r_1 \geq r_2 \cdots \geq r_n$. As mentioned earlier, we will primarily focus on the BundleMVL-2 model, whose expected revenue function can be written more explicitly as:

$$R_2(C) = \frac{\sum_{i \in C} r_i V_i}{v_0 + \sum_{i \in C} V_i} + \sum_{i \in C, j > i} (r_i + r_j) \frac{V_{i,j}}{v_0 + \sum_{i \in W} \sum_{j \in W} \hat{r}_{ij} \theta_{ij} x_i^C x_j^C},$$

where $x_i^C = 1$ if $i \in C$ else 0, $\theta_{ij} = \begin{cases} V_{ij} \quad &i \neq j \\ V_i \quad &i = j \end{cases}$, and $\hat{r}_{ij} = \begin{cases} r_i + r_j \quad &i \neq j \\ r_i \quad &i = j \end{cases}$. Our objective is to find a recommendation set $C^*$ that has the maximum expected revenue among all feasible recommendation sets (represented using collection $C$):

$$\max_{C \in \mathcal{C}} R_2(C).$$

We first consider the unconstrained case, i.e., when $C = 2^W$. We show that this problem is NP-complete, and consequently derive structural properties of the optimal solution that will be used effectively in algorithm design (Section 4.1.1). The case when the collection of feasible recommendation sets is given by linear constraints is tackled in Section 4.2.

3.1. Hardness of Optimization

The revenue functions $R_2(C)$ and $R_K(C)$ have a form similar to the expected revenue of recommendations under the MNL model. For the MNL model, it is known that the unconstrained revenue optimization problem can be solved in linear time as the optimal set is a revenue-ordered set, i.e., it only contains the $l$ highest priced products for some $l \in \mathbb{Z}_+$. But for the BundleMVL-2 model, we show that this does not hold.
Theorem 1. [Hardness Result for BundleMVL-2] Under the BundleMVL-2 model, the decision version of the unconstrained revenue optimization problem \( \textbf{(1)} \) is NP-complete.

The proof of the theorem follows from a reduction of the well-known MAXCUT problem and is given in the appendix. While the existence of a polynomial time approximation algorithm for problem \( \textbf{(1)} \) is an open question, we believe it is inapproximable because it is similar to the quadratic knapsack problem with additional constraints on the coefficients (that can be both positive and negative). And it is known that the quadratic knapsack problem (defined on an edge-series parallel graph) is hard to approximate \( \textbf{(Rader Jr and Woeginger 2002)} \). On a related note, we also provide a similar hardness result for the MMC multi-choice model (proof is in the appendix).

Theorem 2. [Hardness Result for MMC] The decision version of the unconstrained revenue optimization problem under the MMC model (with number of allowed purchases \( \leq 2 \)) is NP-complete.

These results are not surprising given similar results in prior works for single-choice models \( \textbf{(Rusmevichientong et al. 2010b)} \). In the absence of polynomial time exact algorithms for the optimization problem \( \textbf{(1)} \), we can either develop exact algorithms without any run-time guarantees, or create heuristic polynomial time algorithms. We explore both these directions, and improve them based on new structural properties, which we describe next.

3.2. Structural Properties of the Optimal Solution

Under the setting \( C = 2^W \), i.e., for the unconstrained optimization problem \( \textbf{(1)} \), we prove useful structural properties satisfied by the optimal solution \( C^* \) (proofs of these results are in the appendix):

Lemma 2. For all products \( i \in W \) that are not in any optimal recommendation set \( C^* \), \( r_i \leq R_2(C^*) \). Equivalently, \( C_u^* \subseteq C^* \), where \( C_u^* = \{ i : r_i > R_2(C^*) \} \).

Lemma 3. Let \( C^* \) be an optimal recommendation set. For every \( i \in C^* \), \( \exists \ j(i) \in C^* \), where \( j(i) \neq i \) and \( r_i + r_{j(i)} \geq R_2(C^*) \).

Remark: If \( C^* \) is an optimal recommendation set of the smallest cardinality, then \( \forall \ i \in C^* \), \( \exists \ j(i) \in C^* \), where \( j(i) \neq i \) and \( r_i + r_{j(i)} > R_2(C^*) \).
**Lemma 4.** Let the $i$-th revenue-ordered recommendation set be defined as $A_i = \{1,2,\cdots,i\}, i \in W$. Then, the revenue of revenue-ordered recommendation sets increases monotonically as long as the price of all the products in the revenue-ordered recommendation set is greater than $R_2(C^*)$, i.e., $R_2(A_1) \leq R_2(A_2) \cdots \leq R_2(A_k)$ where $r_k > R_2(C^*) \geq r_{k+1}$.

Lemma 2 says that if a product’s revenue is greater than the optimal revenue, then it belongs to the optimal recommendation set. Lemma 3 suggests that a product that is in the optimal recommendation set has a corresponding pair that also belongs to the optimal set such that the sum of their revenues is greater than the expected revenue of the set. Finally, Lemma 4 suggests that the objective function has a partial monotonicity property. Overall, these three properties can help us narrow the search for the optimal recommendations. For instance, if an algorithm keeps an estimate of an upper bound on the optimal revenue, then this can help prune the search space based on Lemma 2.

4. Algorithms for Revenue Maximizing Recommendations

We propose a new algorithmic approach for solving problem (1). We first consider the unconstrained problem i.e. when $C = 2W$ and then consider the setting with linear constraints. Our approach is based on binary search and outputs recommendations having revenue within a specified range of the optimal revenue. The iterative nature of this approach helps in terminating the search for the optimal recommendations gracefully, especially under stringent timing requirements expected in personalization focused applications on e-commerce platforms. We also consider three benchmark methods for the same optimization problem - one of which gives the optimal solution and the other two are heuristic. We discuss structural properties of the solutions obtained by the heuristic algorithms and examine conditions under which they can be optimal.

4.1. Binary Search with Efficient Comparisons

A binary search based efficient algorithm for a single-choice model was first described in Sinha and Tulabandhula (2020), who evaluate the efficacy of using nearest neighbor search techniques for capturing arbitrary feasibility constraints in the comparison step. Building on their algorithmic strategy, we devise a binary search outer loop and focus on improving the computational speed of
the comparison steps by exploiting the structure of our multi-purchase choice model. While such a use of the binary search template is common for transforming optimization problems to feasibility problems (and vice versa), we show below that in our context this allows for two key efficiency gains, namely: (a) use of structural properties reduces search space significantly, and (b) allows for extensively developed heuristics for the comparison step giving us scalability. For any given tolerance $\epsilon > 0$, this algorithm gives an $\epsilon$-optimal solution, i.e., a solution within $\epsilon$ of the optimal value. In each iteration of the search process, we narrow the size of the interval in which $R(C^*)$ lies as outlined in BinarySearchAO (Alg. 1). The computationally expensive comparison step (COMPARE-STEP, line 4 in Alg. 1) checks if the optimal revenue is greater than the specified threshold $\kappa_j$. A key insight is that this calculation can be transformed as follows:

$$\max_{C \in C} R(C) \geq \kappa_j \iff \max_{C \in C} \sum_{i \in W} \sum_{j \in W} \theta_{ij} x_i^C x_j^C (\hat{r}_{ij} - \kappa_j) \geq \kappa_j v_0. \tag{2}$$

The optimization problem on the left hand side of the transformed comparison is a quadratic integer program (QIP). In the absence of constraints (e.g., capacity constraints), this problem is a member of a specialized class of QIP problems known as Quadratic Unconstrained Binary Optimization (QUBO) problems, which are known to be NP-hard (Pardalos and Jha 1992). Although the set of all comparison step (QIP) instances is a strict subset of the QUBO instances, for simplicity we will refer to the comparison step instance as a QUBO instance when the context is clear. The binary search template can also be used to solve other BundleMVL-K models (the COMPARE-STEP will be different), and Section 5 documents its use with the BundleMVL-3 model.

4.1.1. Using Structural Properties of $C^*$: BinarySearchAO can be made more efficient by using the properties of the optimal recommendation set derived earlier (Lemma 2). At the cost of additional pre-processing (which is small), we can start with a lower bound greater than 0 based on Lemma 4. Let $l$ be the maximum index $i$ such that $R(A_1) \leq R(A_2) \cdots \leq R(A_i)$. Then, from Lemma 4 we know that $l \geq k$ (see the definition of $k$ in the Lemma). Thus, $r_k \geq R(C^*) \geq r_{k+1} \geq r_{l+1}$. Hence, at the beginning of the binary search, the lower bound $L$ can be set as $r_{l+1}$. 
### Alg. 1 BinarySearchAO

**Require:** Parameters \( \{r_i\}_{i=1}^n, \{\theta_{ij}\}_{i=1,j=1}^n \),

tolerance level \( \epsilon > 0 \), and feasible sets \( C \).

1: \( L_1 = 0, U_1 = r_1 + r_2, j = 1, \) and \( C^* = \{1\} \).

2: **while** \( U_j - L_j > \epsilon \) **do**

3: \( \kappa_j = (L_j + U_j)/2 \).

4: **if** \( \kappa_j \leq \max_{C \in C} R(C) \) **then**

5: \( L_{j+1} = \kappa_j, U_{j+1} = U_j \).

6: Pick any \( C^* \in \{C \in C : R(C) \geq \kappa_j\} \).

7: **else**

8: \( L_{j+1} = L_j, U_{j+1} = \kappa_j \).

9: Increment \( j \) by 1.

10: **return** \( C^* \)

### Alg. 2 BinarySearchAO(Efficient)

**Require:** Parameters \( \{r_i\}_{i=1}^n, \{\theta_{ij}\}_{i=1,j=1}^n \),

tolerance level \( \epsilon > 0 \), and feasible sets \( C \).

1: \( U_1 = r_1 + r_2, j = 1, i = 1 \) and \( C^* = \{1\} \).

2: **while** \( r_{i+1} \geq r_i \) **do** Increment \( i \) by 1.

3: \( L_1 = r_{i+1} \).

4: **while** \( U_j - L_j > \epsilon \) **do**

5: \( \kappa_j = (L_j + U_j)/2 \).

6: **if** \( \kappa_j \leq \max_{C \in C} R(C) \) **then**

7: \( L_{j+1} = \kappa_j, U_{j+1} = U_j \).

8: Pick a \( C^* \) such that \( R(C^*) \geq \kappa_j, \overline{B} \subset C^* \), and \( \overline{B} \cap C^* = \emptyset \); where \( \overline{B} = \{i : r_i > U\} \), and \( \overline{B} = \{i : r_i + r_1 < L\} \).

9: **else**

10: \( L_{j+1} = L_j, U_{j+1} = \kappa_j \).

11: Increment \( j \) by 1.

12: **return** \( C^* \)

Lemmas 2 and 3 can be used to make the comparison step faster. In particular, when we have an upper bound \( U \) on \( R(C^*) \), then using Lemma 2 we know that all products with revenue greater than \( U \) should belong to the optimal recommendation set. Similarly, with a lower bound \( L \) on the revenue of the optimal recommendation set, we know that all products \( i \) such that \( r_i + r_1 < L \), cannot belong to the optimal recommendation set. These observations predetermine the fate of some products, reducing the problem size (sometimes significantly as seen in our experiments) in the comparison step 2. BinarySearchAO(Efficient) incorporates these properties is shown in Algorithm 2.
4.1.2. Solving the QUBO Problem Approximately: Though the QUBO problem is an NP-hard problem \cite{Pardalos1992}, as discussed before, there has been ample research in heuristic algorithms that return high quality solutions in extremely reasonable computation times \cite{Dunning2018}. This makes it appealing to use these approximate algorithms in solving the COMPARE-Step. Nonetheless, solving problem (2) approximately can potentially lead to narrowing down on an incorrect interval in the binary search outer loop. We take two steps to alleviate this issue:

Firstly, for each QUBO problem, we run multiple QUBO heuristics in parallel, as seen in our experiments (Section 5). The binary search interval will have an incorrect update only if all the heuristics lead to an incorrect answer for the COMPARE-Step. Secondly, we further robustify the binary search outer loop by using a noisy binary search variant \cite{Burnashev1974}. Here one maintains a distribution over the unknown $R(C^*)$, and each comparison (with the median of the current distribution) is used to obtain an updated distribution using Bayes rule. This prevents incorrect comparison step outcomes from easily misleading the search process. For any specified tolerance level and a probability value with which the given solution needs to lie within the tolerance level, the number of iterations required for the noisy binary search still stays logarithmic. We refer to this algorithm as NoisyBinarySearchAO and its version which uses the structural properties as NoisyBinarySearchAO(Efficient) (we omit its description due to space constraints).

4.2. Optimization with Linear Constraints

Constraints on the feasible recommendation sets are common in practice. For example, there can be a cardinality constraint on the maximum number of products in a recommendation set due to webpage/screen size limits in the online e-commerce setting, or due to limited shelf space in the offline retail setting. Business rules and obligations such as ensuring sufficient representation from various sub-groups of products, or the requirement to maintain a precedence order among products can also be formulated as linear constraints \cite{Davis2013,Sinha2020}. The binary search algorithm (Algorithm 1) can incorporate linear constraints in the following way. For a general linear constraint set $Dx = e$, the COMPARE-STEP becomes

$$\max_{\{x \in \{0,1\}^n : Dx = e\}} \sum_{i \in W} \sum_{j \in W} \theta_{ij} x_i x_j (\hat{r}_{ij} - \kappa) \geq \kappa v_0.$$
This is a quadratic binary optimization problem with constraints that can be relaxed to get
\[
\max_{x \in \{0, 1\}^n} \sum_{i \in W} \sum_{j \in W} \theta_{ij} x_i x_j (\hat{r}_{ij} - \kappa) + \lambda (Dx - e)'(Dx - e),
\]
for a suitably large \( \lambda < 0 \). In this form, the aforementioned QUBO solvers can be used directly.

If we have an inequality constraint, then as long as the components of \( D \) and \( e \) are integral, a similar transformation can be done with an appropriate number of slack variables (Glover and Kochenberger 2018). For instance, suppose we want to ensure that the size of the recommendation set is at most \( e \in \mathbb{Z}_+ \), i.e., we have the constraint \( \mathbf{1}'x \leq e \) (here, \( \mathbf{1} \) is the vector of all ones). Then, using slack variables \( s_1, ..., s_e \), we get the following readily solvable QUBO instance:
\[
\max_{x \in \{0, 1\}^n} \sum_{i \in W} \sum_{j \in W} \theta_{ij} x_i x_j (\hat{r}_{ij} - \kappa) + \lambda (\mathbf{1}'x + \sum_{i=1}^e s_i - e)'(\mathbf{1}'x + \sum_{i=1}^e s_i - e).
\]
(3)

### 4.3. Benchmark Algorithms

We briefly describe three benchmark algorithms we considered - one of which is an exact algorithm, and the other two are heuristics extending exact algorithms for some single-choice models.

The first benchmark is based on a mixed integer program (MIP) formulation and gives an exact solution. This formulation builds on an earlier formulation for the mixture of MNLs model studied in Blanchet et al. (2016), and is described in Algorithm 4 in the appendix. This benchmark can also easily incorporate linear constraints mentioned above.

Our next benchmark is a generalization of the Adxopt algorithm (Jagabathula 2014), called the AdxoptL algorithm (Alg. 5 in the appendix, \( L \) is a parameter). This is a choice model agnostic greedy algorithm which in every iteration looks for a set of \( L \) products whose addition/deletion/exchange will lead to recommendations with a higher revenue. The solution \( \hat{C} \) of Adxopt2 (i.e., \( L=2 \)) is guaranteed to contain all relevant high-revenue products as per the below lemma (proof in appendix).

**Lemma 5.** Let \( \hat{C} \) be the solution returned by Adxopt2 using the BundleMVL-2 model. Then, \( \hat{C} \supset C_u^* \), where \( C_u^* = \{ i : r_i > R_2(C^*) \} \).

The (worst-case) time complexity of the Adxopt2 algorithm is \( O(n^7) \), which is prohibitive for medium to large instances as observed in our experiments.
Our third benchmark is a heuristic algorithm which chooses the revenue-ordered recommendation set with the highest revenue, and has a time complexity of $O(n^3)$. This heuristic is known to be optimal or close to optimal for several single-choice models [Rusmevichientong et al. 2010b]. In what follows, we characterize conditions under which this heuristic performs well for the BundleMVL-2 model, by generalizing the notion of value conscious customers introduced in [Rusmevichientong et al. 2014] to our multi-purchase setting. These customers prefer a cheaper product (or pair of products) when compared to a more expensive product (or pair of products) but derive more value from a higher priced product (or pair of products). Here value is defined as the product of the revenue and the utility parameters associated with the set of purchased items. This intuition is formalized below:

**Assumption 1.** Model parameters for value conscious customers satisfy:

(a) $V_{\{i\}} \leq V_{\{j\}} \text{ and } V_{\{i,k\}} \leq V_{\{j,k\}} \forall i < j, i \neq k, j \neq k$ and $i, j, k \in W$

(b) $r_i V_{\{i\}} \geq r_j V_{\{j\}} \text{ and } (r_i + r_k) V_{\{i,k\}} \geq (r_j + r_k) V_{\{j,k\}} \forall i < j, i \neq k, j \neq k$ and $i, j, k \in W$.

**Theorem 3.** For value conscious customers, the revenue-ordered heuristic produces an optimal recommendation set for the optimization problem $\max_{|C| \leq d} R_2(C)$ for any $d > 0$.

When all the $V_{\{i,j\}}$ values are 0, the BundleMVL-2 model reduces to an MNL model, and the optimal recommendation set is a revenue-ordered recommendation set for the unconstrained optimization problem. This gives us another set of conditions where we can show that the revenue-ordered heuristic produces good solutions, namely when the $V_{\{i,j\}}$ values are small compared to $V_{\{i\}}$ values:

**Assumption 2.** Model parameters satisfy: $\max_{i,j \in W, i \neq j} V_{\{i,j\}} \leq \epsilon \min_{k \in W \cup \emptyset} V_{\{k\}}$.

**Theorem 4.** Under Assumption 2, the revenue-ordered heuristic satisfies: $R_2(C^*_{\text{revord}}) \geq \frac{2 - \epsilon}{2 + 4\epsilon} R_2(C^*)$, where $C^*_{\text{revord}} \in \arg \max_{C \in \{A_1, A_2, \ldots, A_n\}} R_2(C)$, and $C^*_{\text{MNL}}$ and $C^*$ are the optimal solutions of the unconstrained problem under the MNL and the BundleMVL-2 models respectively.

We note in passing that guarantees similar to the above can be obtained for Binary-SearchAO(Efficient) if we can obtain an approximation guarantee for the Compare-Step under the same assumptions. We omit this analysis here for brevity, and shift our attention to evaluating the value of modeling multiple purchases and of our algorithms using real datasets next.
5. Experiments

We perform two sets of experiments. The goal in the first set is to validate the merits of the BundleMVL-2 model compared to other models on real data based on the empirical fit and the revenue obtained by optimizing based on this model. In the second set, we benchmark the solution quality and computational times of the optimization approaches (Section 4) in detail, to ascertain their suitability in offline and online recommendation settings.

All results reported here are based on 50 Monte Carlo runs for each configuration, unless otherwise noted. For computation times and the optimality gap metrics, we have plotted the median along with the 25th and 75th percentiles. We segment the number of products \( n \) into three regimens, viz., (a) Small: 20 – 80, (b) Medium: 100 – 400, and (c) Large: 500 – 1500 products, while discussing scalability trends. Additional runs/variations of these experiments are documented in the appendix.

5.1. Suitability of the BundleMVL-2 Model on Real Data

We perform two assessments: (a) the fit of the BundleMVL-2 model on real world datasets, and (b) the revenue gains that can be achieved with this model compared to other competing models.

5.1.1. Empirical Fit of BundleMVL-2 vs Others: We compare the BundleMVL-2 model with the MMC and the MNL models. For this, we use five datasets (Bakery, Walmart, Kosarak, Instacart, LastFMGenres) that have fixed recommendation sets across all interactions, and one dataset from YOOCHOOSE (two variants ycItems and ycDepts) that has variable recommendation sets (see Benson et al. (2018) for their descriptions). While some of these are not explicitly about purchases, they do capture multi-choice behavior of consumers. Additionally, we also use the Ta Feng Grocery (https://www.kaggle.com/chiranjivdas09/ta-feng-grocery-dataset) and the UCI Online Retail (https://archive.ics.uci.edu/ml/datasets/online+retail) datasets that contain information about the revenues/prices in addition to the bundles purchased in the subsequent sections. These datasets are from a variety of domains, and Table 2 summarizes the relevant characteristics. We filter these datasets to transform all observations into ones that involve at most two-sized bundle purchases (see appendix), after removing extremely infrequent products (\(~ 10\% \) on average).
All datasets are split in the ratio 80:20, with the former used for learning the parameters, and the latter for reporting out-of-sample log-likelihood fit. As these datasets do not contain information about customers seeing the recommendation set but leaving without making any purchase, it is not possible to estimate \( v_0 \). Consequently, we rely on domain knowledge to pick an appropriate value in our experiments although this has been observed to vary wildly from one application to another. While the BundleMVL-2 and MNL have no tunable parameters, we need to pick the number of corrections for the MMC model. Increasing the number of corrections increases the flexibility of this model, but also increases the number of parameters. While adding such corrections, we pick bundles (namely the H-sets) in descending order of their frequency of appearance in the datasets (this heuristic is provided in Benson et al. (2018)).

The fit of the three models are tabulated for the two Walmart datasets (also see Figure 1 in Section 1) in Table 3 and for the other six datasets (omitting Ta Feng and UCI) in Table 6 in the appendix. The number of corrections in MMC model have been reported as a percentage (between 0% to 100%) of the number of unique subsets of purchases of size greater than one that are observed. The column \(#\text{parameters}\) denotes the number of non-zero parameters in each model. The number of parameters in BundleMVL-2 differs from MMC with 100% corrections because of the way these are estimated, which leads to different numbers of parameters ending up non-zero in each case. The columns \(\text{train\_ll}\) and \(\text{test\_ll}\) contain the train and test log likelihood values respectively. We fit the MNL and BundleMVL-2 model based on MLE. For the case where the recommendation sets are the same across observations, the parameter estimates can be obtained analytically. In the general case, we use stochastic gradient descent with sane defaults. From these two tables, we infer that the BundleMVL-2 model provides the best fit (i.e., the highest log-likelihood value) in seven of the eight datasets, when compared to the MNL model and the MMC models with different levels of corrections.
The gap between the BundleMVL-2 and MMC models when compared to the single-choice MNL model is quite large (up to $1.5 - 2 \times$ lower log-likelihoods for the latter in some cases), validating the necessity for multi-purchase choice modeling. In summary, for all eight datasets, the BundleMVL-2 model is shown to be a viable and strong alternative to competitors (e.g., the MMC model) in capturing the rich multi-purchase behavior exhibited.

5.1.2. Revenues and Run-times with BundleMVL-2: Even though the BundleMVL-2 model provides a good fit on real data, one of the primary goals of using such choice models in practice is to realize higher expected revenues, and this is our focus next. To start, we estimate parameters of the competing models using the Ta Feng and the UCI datasets. Next, we randomly sample (without replacement) a subset of products of pre-specified sizes, and define a choice model instance using their estimated parameter values. As there is no information about customer interactions that did not lead to a sale in these datasets, we fix the probability of no-purchase when all products are displayed to 30% (changing this probability to much higher and lower values while experimenting did not qualitatively change our conclusions), and estimate the $v_0$ parameter accordingly for each instance.

We perform three comparisons: (1) revenue of BundleMVL-2 vs MNL, (2) revenue and run-times of BundleMVL-2 vs BundleMVL-3, and (3) run-times of BundleMVL-2 vs MMC. When doing these comparisons, we also study their trends as a function of the instance size (i.e., number of products $n$).

Comparison (1): Revenue of BundleMVL-2 vs MNL: Since the MNL model is a special case of the BundleMVL-2 model, we take the BundleMVL-2 model to be the ground truth, and calculate final revenues based on this. The optimality gap (which is the percentage difference from the optimal under ground truth) of the optimal assortment under the MNL model is shown in Figure 2a. Here, we
Figure 2  Performance plots. (a): Optimality gap of the optimal recommendation set as per the MNL model with the ground truth as the BundleMVL-2 model. (b): Time taken to solve for the optimal recommendation set for the unconstrained optimization problem under different models. (c): Optimality gap of the optimal recommendation set under the BundleMVL-2 model with the BundleMVL-3 model as the ground truth. (d): Time taken to solve the unconstrained optimization problem under different models. Ta Feng-BundleMVL-2 and UCI-BundleMVL-2 run-times overlap. (e): Assessing optimality of revenue-ordered heuristic.

observe that this optimality gap increases as the number of products increase. Moreover, it becomes significant for large product sizes. Thus, modeling purchase of multiple products (for instance, by using BundleMVL-2) can lead to significant revenue gains if we can also improve run-times of these models. For instance, since optimization over MNL is linear time, it is important to bring down the computational complexity of optimization over BundleMVL-2 model, and we investigate this exhaustively in Section 5.2.

Comparison (2): Revenue and run-times of BundleMVL-2 vs BundleMVL-3: Previously, we made a remark that a significant portion of observed bundles are of size at most two in many real datasets
and that the optimization problem becomes more challenging as $K$ increases. Here, we compare if the potential revenue gains by using a richer model can trade-off the increase in computation. The setup is similar to the previous comparison. Here, the revenues are reported using the estimated BundleMVL-3 model as the ground truth model. In order to optimize over BundleMVL-3 model, we use a mixed non-linear integer programming solver called Bonmin from COIN-OR (Bonmin). BinarySearchAO algorithm is used to solve for the optimal recommendation set under both models. Figure 2c shows the optimality gap of the BundleMVL-2 model. These optimality gaps are much smaller than the gaps observed in the BundleMVL-2-MNL comparison. Further, the time taken to perform the optimization increases dramatically for BundleMVL-3 as seen in Figure 2d. This likely stems from the difficulty in solving cubic integer optimization problems as compared to quadratic integer optimization problems. Thus, the revenue gains are small and do not outweigh the computational burden of optimizing over the BundleMVL-3 (and other BundleMVL-K models for $K > 3$) for large scale applications.

Comparison (3): Run-times of BundleMVL-2 vs MMC: A direct comparison of the revenues obtained using the BundleMVL-2 and MMC models is difficult because neither of the models are nested within the other. Moreover, a reasonable parsimonious multi-choice model that has both these models as special cases is hard to construct. Thus, we restrict our attention to comparison of run-times for computing the optimal recommendation set. To keep the comparison fair, we solve the corresponding integer programming formulation (see appendix) for each setting. Based on Figure 2b, we can conclude that the run-time is much faster under the BundleMVL-2 model, making it a better candidate for large-scale/time-constrained applications. Moreover, we demonstrate in the next subsection that solutions for the BundleMVL-2 model can be obtained even faster using the proposed binary search algorithms.

5.2. Run-times for Computing BundleMVL-2 based Recommendation Sets

We now focus on the BundleMVL-2 model and benchmark the computation times and quality of solutions produced by various algorithms described in Section 4 on the TaFeng and UCI datasets.
Similar evaluations for the MMC model is presented in the appendix. To get problem instances of different sizes, we use a similar procedure as described before wherein we learn parameters for the full dataset and then subsample the desired number of products and their respective parameters. For the following list of experiments designed to illustrate how scalable our proposed algorithmic approaches are, we report results for the Ta Feng dataset and relegate results for the UCI dataset (which has similar trends as Ta Feng) to the appendix:

1. Selecting QUBO heuristics for the BundleMVL-2 model,
2. Benchmarking algorithms for the BundleMVL-2 model (unconstrained setting),
3. Benchmarking algorithms for the BundleMVL-2 model (constrained setting), and
4. Assessing optimality of the revenue ordered heuristic for the BundleMVL-2 model.

1. **Selecting QUBO heuristics for the BundleMVL-2 model:** As discussed in Section 4, we can use efficient approximate algorithms to solve the QUBO problem in conjunction with a (noisy) binary search outer loop to accelerate the search. Many heuristics have been proposed in the literature for solving the QUBO problem (Boros et al. 2007). We evaluate these heuristics to decide which ones to use in the NoisyBinarySearchAO algorithm.

   To start with, we consider ~20 heuristics discussed in Dunning et al. (2018) (https://github.com/MQLib/MQLib), and solve several QUBO instances of the COMPARE-STEP stemming from optimizing over synthetically generated BundleMVL-2 models. Results show that none of the heuristics consistently outperform others in terms of solution quality. Thus, we measure the performance of each heuristic in terms of the proportion of times it gave the best solution among all heuristics. Table 4 summarizes the performance of the top four heuristics ranked in this manner. For subsequent experiments, we run all these top four heuristics at each comparison step of NoisyBinarySearchAO, and then select the best solution to resolve the comparison more accurately. Since the heuristics can be run in parallel, there is no significant increase in time taken as compared to using a single heuristic.

2. **Benchmarking algorithms for the BundleMVL-2 model (unconstrained setting):** Next, we benchmark our proposed and other competing approaches when there are no constraints on the feasible
recommendation sets. Table 5 summarizes the list of algorithms that we consider in various product size regimes. The regimes in which each algorithm can be tested is decided based on the run-time and memory requirements of the algorithm. The MIP formulations are solved using CPLEX version 12.9.0 while the others are based on Python 3.7.4/Numpy 1.17, with some custom C++ code for the QUBO heuristics. We rely on two measures: (a) the fraction of times the algorithm generates a suboptimal solution, and (b) median optimality gap over all Monte Carlo runs. Utilizing structural properties improves solution quality and leads to faster computations because number of products to optimize over in subsequent Compare-Steps keeps decreasing. Thus, we use BinarySearchAO(Efficient) instead of BinarySearchAO for this experiment.

Figures 3a, 3b and 3c, 3d show the fraction of times suboptimal solutions were returned and the optimality gap of various algorithms respectively. From these plots, we note that NoisyBinarySearchAO(Efficient) has good performance on all instance sizes. It converges to the optimal solution for more than 90% of the instances for all regimes of product sizes. We also note that the other heuristic approaches - the revenue-ordered heuristic, Adxopt and Adxopt2 - also output close to optimal solutions, even though the revenue-ordered heuristic fails to return an optimal solution most of the time.

Next, we compare the run-times of these algorithms in Figures 3e and 3f. We observe that the run-time of the two greedy algorithms (Adxopt and Adxopt2) and also the MIP solver doesn’t scale well as the number of products increases. Moreover, the greedy algorithms have a large variance in run-times. Consequently, we limit their evaluation to the small regime (where the number of products
Figure 3  Optimality gap and run-time analysis for the unconstrained optimization problem on the Ta Feng dataset.

Fraction of suboptimal solutions: In (a), BinarySearchAO(Efficient), NoisyBinarySearchAO(Efficient), Adxopt2 and Adxopt return no suboptimal solution when number of products $n \leq 60$. In (b), revenue-ordered heuristic seems to trail in terms of obtaining optimal solutions. Optimality gap: In (c), all the algorithms have the median optimality gap as 0. In (d), BinarySearchAO(Efficient) and NoisyBinarySearchAO(Efficient) curves overlap and very close to 0. Also, the gaps for revenue-ordered are small in the context of this dataset. Run-times: In (e) Adxopt, MIP, BinarySearchAO and revenue-ordered curves are close to zero, but they increase a lot for larger sizes. In (f) we see that revenue-ordered heuristic is much faster as expected.

is less than 100). Among the binary search based approaches, NoisyBinarySearchAO(Efficient) becomes faster in comparison to exact binary search as number of products increase. Also, as expected, the revenue-ordered heuristic takes the least time to run. Overall, the binary search and revenue-ordered algorithms scale well as the number of products increase when compared to other approaches. Between binary search approaches and the revenue-ordered heuristic, the former have a lower optimality gap (with direct implications on expected revenue). While one could make a case about trading-off sub-optimality with speed in favor of the revenue-ordered heuristic, we illustrate
later in this section how the heuristic’s performance is very sensitive to the datasets. In particular, it exhibits large optimality gaps for some natural synthetically generated datasets.

3. Benchmarking algorithms for the BundleMVL-2 model (constrained setting): In this experiment, we evaluate the performance of algorithms when there is a constraint on the size of the feasible recommendation set. The Adxopt and Adxopt2 heuristics are modified so that in every greedy step, the best subset of products to add is chosen while ensuring that the capacity constraint is obeyed. Similarly, for the revenue-ordered heuristic, we choose the best among all revenue-ordered sets of size less than the given capacity. The structural properties of the optimal solution under the unconstrained setting do not hold for the capacitated setting. Thus, we do not use the efficient versions of our binary search approach, and focus our evaluation to small and medium regimes of number of products. We fix the capacity constraint to 5 and 20 for these two regimes respectively.

Further, to use heuristic QUBO solvers, we need to reformulate the optimization problem with capacity constraint to an unconstrained optimization problem as described in Equation (3). Empirically, we observe that the heuristic QUBO solvers don’t perform well in this setting. One reason for why this happens is the following: in the unconstrained setting, we observe that the value of $\theta_{ij}$ is 0 or close to 0 for many pairs of products. As a result, the quadratic coefficient matrix is sparse, and moreover has small values in the entries where the coefficient is non-zero. In the capacity constrained problem, we add an additional term to the objective with the scalar multiplier $\lambda$ taking a large negative value. Thus, all the coefficients become non-zero. This significantly changes the sparsity of the problem instance, giving us poor quality solutions when solved using the previously shortlisted QUBO heuristics.

The performance of different algorithms is presented in Figure 4. As discussed, the noisy binary search approach that uses heuristics does much worse in terms of solution quality as compared to binary search using an exact QUBO solver. Also, there is no significant improvement in solution quality as compared to the revenue-ordered heuristics for this dataset. Due to the capacity constraint, the greedy algorithms Adxopt and Adxopt2 also run much faster (when compared to their performance
Optimality gap and run-time analysis for the optimization problem with capacity constraints on the TaFeng dataset. (a): BinarySearchAO, MIP and Adxopt gets optimal solution in most runs, i.e the plots overlaps near zero value. (b) and (d): NoisyBinarySearchAO uses the revenue-ordered solution as a lower bound and generates no gain on top of it. The curves overlap completely. (c): Adxopt, Adxopt2, MIP and BinarySearchAO plots overlap as the median optimality gap is zero in the small product size regime. Revenue-ordered’s gap improves from (c) to (d) due to an increase in the capacity constraint.

in the unconstrained setting). The revenue-ordered algorithm has a constant time performance as it only needs to evaluate the first $d$ revenue-ordered sets where $d$ is the capacity constraint, irrespective of the total number of products. Overall, we conclude that the current shortlisted QUBO heuristics are not competitive for this constrained setting when compared to other approaches. Nonetheless, the binary search approach works well with exact computation at each comparison step. It also scales well in this product size regime. We will need newer heuristics to improve the run-time if the binary search approach needs to compete with other approaches (revenue-ordered, Adxopt or Adxopt2) in larger product size regimes.
4. Assessing optimality of the revenue-ordered heuristic for the BundleMVL-2 model: In both the settings above, i.e., the unconstrained and the constrained optimization over the Ta Feng, as well as with the UCI dataset in the appendix, we observe that the revenue-ordered heuristic performs quite well both in terms of run-time and optimality gap. In both these datasets, the proportion of non-zero $\theta_{i,j}$s is $\sim 2\%$, which explains the efficacy of the heuristic based on our analysis (see Thm. 4). Motivated by this observation, we further test the performance of this heuristic on additional synthetically generated datasets, and observe that the optimality gap of this heuristic is not always as low as in the two real world datasets we considered before. One such synthetic data generation process for the BundleMVL-2 model is as follows: we divide the products into two groups of equal size - high priced products and low priced products. Users are very unlikely to buy two high priced products. To capture this, $\theta_{i,j}$ parameters are sampled from Beta(1, 10) distribution when products $i$ and $j$ both belong to the high priced group, and the rest of the $\theta_{i,j}$s are sampled from Beta(10, 1) distribution. Additionally, the prices ($r_i$'s) are sampled from Beta(2, 10) and the $\theta_i$ parameters are sampled from Beta(1, 1).

Figure 2e shows the optimality gap of revenue-ordered and NOISYBINARYSEARCHAO algorithms on BundleMVL-2 instances of this type, supporting our hypothesis. We observe that the revenue-ordered heuristic has higher optimality gaps as compared to those observed in the experiments with Ta Feng and UCI datasets. This sensitivity to datasets may tip the sub-optimality speed trade-off balance back in favor of our proposed binary search based approaches.

6. Discussion

While the focus of the paper has been on proposing a parsimonious model for multi-purchase behavior in retail and other online settings followed by algorithmic solutions for maximizing revenues, there are a few key managerial insights that become apparent. Firstly, the investigations in this paper support the importance of modeling richer consumer behavior models going beyond what has been done previously. Although operational decision based on these richer models may pose challenges, we have shown fairly extensively that scalable near real-time computation of revenue maximizing recommendation sets is entirely feasible, even if the problem is NP-complete in theory. Not only is
the computation fast, but the expected revenue gains to be had with richer models make them well worth the effort. Second, practitioners should not be afraid of the increase in complexity with these models. For instance, the proposed models in this work are parametric and interpretable, and only depend quadratically on the number of products, a feature common with many single-choice models such as the Markov chain choice model, the paired combinatorial logit model and others.

Third, managers and practitioners can easily trade-off model complexity with increase in optimization times with the models and algorithms proposed here. The richer the model, the better it represents consumer purchase behavior, while at the same time increasing the operational aspects (such as run-times). In fact, the iterative nature of the proposed algorithm allows one to control this trade-off in a fine grained manner: they can choose less number of iteration steps to solve for candidate recommendation sets, which may not be optimal but useful to improve the user experience and revenues compared to the alternative. Further, BundleMVL-2 model from the BundleMVL-K family seems to be rich enough to provide tangible gains when compared to single-choice models.

Fourth, the search for scalable solutions should be a high priority given the level of personalization that consumers expect from these platforms today. Techniques ranging from segmenting products into clusters, or inducing sparsity in the BundleMVL-2 by thresholding smaller $\beta_{ij}$s to zero, can help achieve this goal, in addition to the use of structural properties and heuristics that we demonstrated here. Finally, a key insight useful for decision makers and practitioners that emerged from the experiments conducted in this paper is the remarkable effectiveness of provably suboptimal heuristics on real world data. While theory only gives limited insights on the optimality performance of heuristics such as the revenue-ordered heuristic or ADXOPTL, we empirically observe that they were fairly competitive to the best performing binary search based approach that we proposed for two real world datasets. This implies that one should rely on real world data related to the specific problem at hand while making algorithmic as well as modeling choices. The interpretability and simplicity advantages of these heuristics are an added bonus in this regard.
7. Conclusion

In this work, we evaluated the effectiveness of multi-purchase choice behavior captured via the proposed BundleMVL-K family on improving revenues, and compared it to other state-of-the-art models. Significant gains, of the order of 6–8% relative expected revenue improvement, is observed from incorporating multiple purchases (with 1500 products, as compared to the MNL baselines). This linking between revenue/sales gains and multi-purchase behavior models is a key contribution of our work, as almost all prior work in this area was focused on modeling/estimation compared to revenue maximization (we also showed a relative 17% improvement in likelihood fits across 8 datasets). Although the gains are significant, the optimization problems are much harder than those for single-choice models, so we designed scalable algorithms that allow a practitioner to realize these gains in demanding applications such as e-commerce platforms.

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Appendix A: Data Augmentation before MLE for the BundleMVL-K Model

If we want to estimate a BundleMVL-K model where $K$ is smaller than the size of some purchased bundles in the dataset, then we can pre-process these observations. In particular, we first partition the purchased bundle, which is of size larger than $K$, into subsets of size at most $K$, and augment each such subset as an additional observation. We consider all possible such partitions and assign them equal probability weights (see Algorithm 3). The MLE objective is also updated to incorporate these importance weights.

**Algorithm 3** Dataset Pre-processing

Require: Purchased bundles $\tilde{S}_1, \cdots, \tilde{S}_m$.

$S \leftarrow [\text{ }, \text{ }], \text{ weights } \leftarrow [\text{ }, \text{ }], \text{ } l \leftarrow 1.$

while $l \leq \tilde{m}$ do

if $|\tilde{S}_l| \leq K$ then

$S$.append($\tilde{S}_l$) & weights.append(1).

else

Let $Q_l = \{A = (A_1, \cdots, A_t) : \exists \ l \ s.t.$ $\cup_{j=1}^t A_j = \tilde{S}_l, |A_j| \leq K \ \forall \ 1 \leq j \leq t; \text{ and }$ $A_1, A_2, \cdots, A_t \text{ are pairwise disjoint}\}.$

for $R$ in $Q_l$ do

$S$.append($A$) & weights.append($\frac{1}{|Q_l|}$).

$l \leftarrow l + 1.$

return $S$, weights

**Algorithm 4** MIP Formulation (BundleMVL-2 model)

max $\sum_{i \in W} \sum_{j \in W} \hat{r}_{ij} p_{ij}$

s.t. $p_{ij} \leq x_{ij} \ \forall \ i, j \in W,$

$p_{ij} \leq \frac{V_{i,j}}{v_0} p_{00} \ \forall \ i, j \in W$

$p_{ij} + \frac{V_{i,j}}{v_0} (1 - x_{ij}) \geq \frac{V_{i,j}}{v_0} p_{00} \ \forall \ i, j \in W$

$x_{ii} + x_{jj} - 1 \leq x_{ij} \leq \min(x_{ii}, x_{jj}) \ \forall \ i, j \in W$

$x_{ij} \in \{0, 1\} \ \forall \ i, j \in W$

$p_{00} + \sum_{i \in W} \sum_{j \in W} p_{ij} = 1$

$p_{00} \geq 0 \ \forall \ i, j \in W$
Appendix B: Unconstrained Revenue Optimization under the BundleMVL-2 Model: Hardness Result and Structural Properties of the Optimal Solution

Proof of Theorem 1. Consider the decision version of the unconstrained BundleMVL-2 optimization problem:

$$\max_{C \in 2^W} R_2(C) \geq \kappa \iff \max_{C \in 2^W} \sum_{i \in W} \sum_{j \in W} \theta_{ij} x_i^C x_j^C (\hat{r}_{ij} - \kappa) \geq \kappa v_0$$

(COMPARE-STEP)

We will show that this decision version of the revenue optimization problem under the BundleMVL-2 model is NP-complete by a reduction from Max-Cut to this problem. Without loss of generality, we can assume that revenues of all products is less than $\kappa$ (if not, then these products will be in the recommendation set corresponding to the solution of the optimization problem). Consider a graph $G$ with nodes $\{1, \cdots, m\}$. We obtain a modified graph $G'$ by removing all the self-loops in $G$. Let the adjacency matrix of $G'$ be $A'$. Let $d = (d_1, \cdots, d_m)$ denote a $m$-dimensional vector with the $i$-th entry being the degree of node $i$ in the graph $G'$. Consider the following $(m + 1) \times (m + 1)$ matrix $Q = (0, \frac{d}{d/2 - A'})$ with a generic entry $q_{i,j}$ (in the $i$-th row and the $j$-th column). We index the entries of this matrix starting from 0 and the nodes of the graph starting from 1. Hence, for $i > 0$, the $i$-th column of the $Q$ matrix corresponds to the $i$-th node in the graph $G'$. Consider the optimization problem:

$$\arg\max_{C \in 2^W} \sum_{0 \leq i \leq m} \sum_{0 \leq j \leq m} q_{i,j} x_i^C x_j^C,$$

(4)

with solution $C^*$. This optimization problem is equivalent to the Max-Cut problem on the graph $G$ as shown below. Note that the only positive values $q_{i,j}$ are either in the first row or the first column, hence $x_0^C = 1$.

Now, $\sum_{0 \leq i \leq m} \sum_{0 \leq j \leq m} q_{i,j} x_i^C x_j^C = 2 \sum_{1 \leq i \leq m} q_{i,0} x_i^C + 2 \sum_{1 \leq i \leq m} \sum_{1 \leq j \leq m} q_{i,j} x_i^C x_j^C$

$$= 2 \sum_{j \in C^*} \frac{d_j}{2} - 2E_{G'}(\tilde{C}^*, \tilde{C}^*) = E_G((\tilde{C}^*, \{1, \cdots, m\} \setminus \tilde{C}^*)),$$

where $E_{G'}(C, C')$ represents the number of edges between the set of nodes $C$ and $C'$ in the graph $G'$, and $\tilde{C}^* = C^* \setminus \{0\}$. The final expression equals the number of edges across the cut $(\tilde{C}^*, \{1, \cdots, m\} \setminus \tilde{C}^*)$ in the graph $G$.

We can also see that problem (4) can be transformed into an equivalent COMPARE-STEP problem as follows: choose numbers $\kappa, r_0, r_1, \cdots, r_m$ such that $r_0 > \kappa$ and $\kappa/2 > r_1 > r_2 \cdots r_m > 0$. Let $\theta_{ij} = \frac{n_{ij}}{r_i + r_j - \kappa}$, $0 \leq i, j \leq m$. Thus, the problem of finding the maximum cut on any graph can be transformed to the optimization problem in the COMPARE-STEP of a BundleMVL-2 optimization problem. Moreover, given a solution of the COMPARE-STEP optimization problem, the maximum cut of the corresponding graph is evident. Hence, the decision problem and subsequently the BundleMVL-2 optimization problem are NP-complete. ■
Next, we prove the structural properties satisfied by $C^*$. To start with, we decompose the revenue function as shown in the following lemma.

**Lemma 6.** For two sets $C$ and $C'$ such that $C \cap C'$ is the empty set, we have:

$$R_2(C \cup C') = \alpha R_2(C) + (1 - \alpha)T(C, C'),$$

where $\alpha = \frac{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \alpha_{ij}}{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \alpha_{ij}}$ is a value between 0 and 1, and the function $T(C, C')$ is defined as

$$T(C, C') = \frac{\sum_{i \in C} \sum_{j \in \mathcal{C}} \hat{r}_{ij} \theta_{ij}}{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C}} \theta_{ij} + 2 \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \alpha_{ij} \hat{r}_{ij}} + \frac{2 \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \hat{r}_{ij} \theta_{ij}}{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \theta_{ij} + 2 \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \alpha_{ij} \hat{r}_{ij}}$$

**Proof.**

$$R_2(C \cup C') = \frac{\sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \hat{r}_{ij} \theta_{ij}}{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \theta_{ij}}$$

$$= \left( \frac{\sum_{i \in C} \sum_{j \in \mathcal{C}} \hat{r}_{ij} \theta_{ij}}{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C}} \theta_{ij}} \right) + \left( \frac{2 \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \hat{r}_{ij} \theta_{ij}}{v_0 + \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \theta_{ij} + 2 \sum_{i \in C} \sum_{j \in \mathcal{C} \cup C'} \alpha_{ij} \hat{r}_{ij}} \right)$$

$$= \alpha R_2(C) + (1 - \alpha)T(C, C')$$

Given the above decomposition, the proofs of the Lemmas are provided below.

**Proof of Lemma** Let $i \notin C^*$ such that $r_i > R_2(C^*)$. We know, $R_2(C^* \cup i) = \alpha R_2(C^*) + (1 - \alpha)T(C^*, \{i\})$ for some $0 \leq \alpha \leq 1$ and $r_i > R_2(C^*)$. As $R_2(C^* \cup i)$ is a convex combination of $R_2(C^*)$ and $T(C^*, \{i\})$, it is greater than $R_2(C^*)$, contradicting the optimality of the recommendation set $C^*$.

**Proof of Lemma** Suppose $\exists \ i \in C^*$ such that $r_i + r_j < R_2(C^*) \ \forall \ j \in C^* \setminus i$. This implies that $T(C^* \setminus i, \{i\}) < R_2(C^*)$. We know that $R_2(C^*)$ is a convex combination of $R_2(C^* \setminus i)$ and $T(C^* \setminus i, \{i\})$. Thus, $R_2(C^* \setminus i) > R_2(C^*)$ contradicting the optimality of the recommendation set $C^*$.

**Proof of Lemma** Using (5), we can decompose the revenue of the revenue-ordered recommendation set $A_m$ as $R_2(A_m) = \alpha R_2(A_{m-1}) + (1 - \alpha)T(A_{m-1}, \{m\})$, for some $0 \leq \alpha \leq 1$. Also, note that $T(A_{m-1}, \{m\}) \geq r_m$. Further, $r_m > R_2(C^*)$ for $m \leq k$. Thus, $T(A_{m-1}, \{m\}) > R_2(C^*) \geq R_2(A_{m-1})$ for $m \leq k$. But $R_2(A_m)$ is a convex combination of $T(A_{m-1}, \{m\})$ and $R_2(A_{m-1})$. Thus, $R_2(A_m) \geq R_2(A_{m-1})$ for $m \leq k$.

**Appendix C:** Benchmark Algorithms under the BundleMVL-2 Model

**Proof of Lemma** Using the arguments in proof of Lemma and the local optimality of $\hat{C}$, we have $\hat{C}_u \subset \hat{C}$, where $\hat{C}_u = \{i: r_i > R_2(\hat{C})\}$. As $R_2(\hat{C}) \leq R_2(C^*)$, $C_u \subset \hat{C} \subset \tilde{C}$. ■
Alg. 5 ADXOPTL

Require: Set of all products $W$, maximum number of removals $b$, add/delete size parameter $l$.

1: $C_0 = \emptyset$, removals$(i) = 0 \ \forall i \in W$

2: repeat

3: $C^A \leftarrow \arg\max_{C \in \mathcal{A}} R(C)$, where $C^A = \left\{ C : C \in \mathcal{C}, C = C^t \cup C_{add} \right\}$ for some $C_{add} \subseteq W$ s.t. $|C_{add}| \leq l$, removals$(i) < b \ \forall i \in C_{add}$.

4: $C^D \leftarrow \arg\max_{C \in \mathcal{D}} R(C)$, where $C^D = \left\{ C : C \in \mathcal{C}, C = C^t \setminus C_{del} \right\}$ for some $C_{del} \subseteq C^t$ s.t. $|C_{del}| \leq l$.

5: $C^X \leftarrow \arg\max_{C \in \mathcal{X}} R(C)$, where $C^X = \left\{ C : C \in \mathcal{C}, C = C_{add} \cup C^t \setminus C_{del} \right\}$ for some $C_{del} \subseteq C^t, C_{add} \subseteq W$ s.t. $|C_{del}| \leq l$, removals$(i) < b \ \forall i \in C_{add}$.

6: $C^{t+1} = \arg\max \{ R(C^A), R(C^D), R(C^X) \}$.

7: removals$(i) \leftarrow$ removals$(i) + 1 \ \forall i \in C^t \setminus C^{t+1}$.

8: until $R(C^{t+1}) > R(C^t)$ and removals$(i) < b$ for some $i \in W$.

9: return $C^t$

Proof of Theorem 3 Let $C^*$ be an optimal recommendation set for the above problem. We will construct a revenue-ordered recommendation set which has revenue $R_2(C^*)$. If $C^*$ is a revenue-ordered recommendation set, then the theorem is trivially true. Hence, we focus on the case when $C^*$ is not a revenue-ordered recommendation set. Then, there exists products $l, m$ such that $l \in C^*$ and $m \notin C^*$ for some $1 \leq m < l \leq n$.

Let $\tilde{C} = \{ m \} \cup C^* \setminus \{ l \}$. Thus, we have

$$R_2(\tilde{C}) = \frac{\sum_{i \in C^* \setminus \{ l \}} r_i V_i + \sum_{i \in C^* \setminus \{ l \}} \sum_{j \in C^* \setminus \{ l \}, j > i} (r_i + r_j)V_{i,j} + r_m V_m + \sum_{i \in C^* \setminus \{ l \}, i \neq m} (r_i + r_m)V_{i,m}}{v_0 + \sum_{i \in \tilde{C}} V_i + \sum_{i \in C^* \setminus \{ l \}} \sum_{j \in C^* \setminus \{ l \}, j > i} V_{i,j} + V_m + \sum_{i \in C^* \setminus \{ l \}, i \neq m} V_{i,m}} \geq R_2(C^*)$$

As $C^*$ is an optimal recommendation set, $R_2(\tilde{C}) \leq R_2(C^*)$. Hence, we conclude $R_2(\tilde{C}) = R_2(C^*)$. We can use the above argument repeatedly to construct a sequence of recommendation sets, each having revenue equal to $R_2(C^*)$ until a revenue-ordered recommendation set is obtained.

Prior to giving proof of Theorem 4, we define some notation and lemmas that will be useful. We define

$$R_{MNL}(C) = \frac{\sum_{m = \sum_{i \in C} V_i} r_i}{\sum_{i \in C} V_i}, \quad C_{MNL} \in \arg\max_{C \subseteq C} R_{MNL}(C), \quad C_{record} \in \arg\max_{C \subseteq \{ A_1, A_2, \ldots, A_n \}} R_2(C)$$

and $C^* \in \arg\max_{C \subseteq \mathcal{C}} R(C)$. When $\mathcal{C} = 2^W$, we take $C_{MNL}$ to be a revenue-ordered set.
Although Benson et al. (2018) do not model the no purchase option, one way to incorporate the no-purchase option is to assign a utility to the no-purchase option for each size of the subset that can be chosen. The following problem:

\[
\arg\max_{C \in 2^I} \sum_{i \in C} r_i \frac{V_{(i)}}{2 \left( v_0 + \sum_{i \in C} V_{(i)} \right)} + z_2 \sum_{i,j \in C, i<j} (r_i + r_j) \frac{V_{(i,j)}}{2 \left( v_0 + \sum_{i \in C} V_{(i)} \right)} + \sum_{k,l \in C} V_{(k,l)} = (2\text{-PRODUCTS MMC AO})
\]

where \(z_1, z_2\) are the probability of purchasing one and two products respectively such that \(z_1 + z_2 = 1\).

Although Benson et al. (2018) do not model the no purchase option, one way to incorporate the no-purchase option is to assign a utility to the no-purchase option for each size of the subset that can be chosen. The no-purchase option is then treated as an alternative which is always present irrespective of the recommendation set and is represented with the parameters \(V_{(0)}\) and \(V_{(0,0)}\). To establish the NP-completeness of 2-PRODUCTS MMC AO, we use the fact that revenue optimization under the mixture of two multinomial logits (2-CLASS LOGIT AO) is NP-complete (Rusmevichientong et al. 2010b). This optimization problem is:
\[
\arg\max_{C \in 2^W} \alpha_1 \sum_{i \in C} s_i \frac{v_i^1}{v_0^1 + \sum_{j \in C} v_j^1} + \alpha_2 \sum_{i \in C} s_i \frac{v_i^2}{v_0^2 + \sum_{j \in C} v_j^2},
\]

(2-CLASS LOGIT AO)

where the revenues of products are given by \(s_i, \ldots, s_n\) with \(s_i \in \mathbb{Z}_+ \forall i \in [n]\), the preference weights are \((v_0^g, v_1^g, \cdots v_n^g)\) with \(v_i^g \in \mathbb{Z}_+ \forall i \in [n]\), \(g = 1, 2\), and the probability of a customer belonging to each of the mixture components is \((\alpha_1, \alpha_2)\) with \(\alpha_g \in \mathbb{Q}_+, \ g = 1, 2\) and \(\alpha_1 + \alpha_2 = 1\). We claim that there is a reduction from a 2-CLASS LOGIT AO instance to a 2-PRODUCTS MMC AO instance and prove this in two steps:

1. Transform an instance of 2-CLASS LOGIT AO to an instance of 2-PRODUCTS MMC AO: Given an instance of 2-CLASS LOGIT AO, we define an instance of 2-PRODUCTS MMC AO by including an additional \((n+1)\)-th product, which we refer to as a snowball. The revenues of the products in the transformed instance are same as their original revenue and the snowball has zero revenue i.e. \(r_i = s_i \ \forall i \in [n]\) and \(r_{n+1} = 0\). The probability of purchasing one and two products is equal to the probability of belonging to each group i.e. \(z_g = \alpha_g, g = 1, 2\). The preference weights in the transformed instance are given as:

(a) \(V_i = v_i^1 \ \forall i \in \{0, 1, \cdots, n\}\) and \(V_{n+1} = 0\)

(b) \(V_{i,j} = v_i^2\) if \(i = 0, j = 0; v_i^2\) if \(j = n + 1, i \in [n]; v_j^2\) if \(i = n + 1, j \in [n]; 0\) else.

2. Given a solution \(S^*\) of the above instance of 2-PRODUCTS MMC AO obtain a solution for the original instance of 2-CLASS LOGIT AO: this can be done using Lemma 10.

Thus, any instance of the 2-CLASS LOGIT AO can be reduced to an instance of 2-PRODUCTS MMC AO, proving that 2-PRODUCTS MMC AO is also NP-complete. ■

**Lemma 10.** If \(S^*\) is the solution for the above instance of 2-PRODUCTS MMC AO, then \(S^*/\{n+1\}\) is optimal for the 2-CLASS LOGIT AO problem.

**Proof.** It is easy to see that \(R_{MMC}(S) \leq R_{MMC}(S \cup \{n+1\}) \ \forall S \in 2^W\). Thus, without loss of generality, \(n+1 \in S^*\). We define \(R_{MMNL}(S) = \alpha_1 \sum_{i \in S} s_i \frac{v_i^1}{v_0^1 + \sum_{j \in S} v_j^1} + \alpha_2 \sum_{i \in S} s_i \frac{v_i^2}{v_0^2 + \sum_{j \in S} v_j^2}\). Thus, with the parameters specified as above, \(R_{MMNL}(S) = R_{MMC}(S \cup \{n+1\}), \ \forall S \in 2^W\). Assume \(\tilde{S} \neq S^*/\{n+1\}\) is the solution for 2-CLASS LOGIT AO. Thus, \(R_{MMC}(\tilde{S} \cup \{n+1\}) = R_{MMNL}(\tilde{S}) > R_{MMNL}(S^*) = R_{MMC}(S^*)\) contradicting the assumption that \(S^*\) is the solution to 2-PRODUCTS MMC AO. ■
Figure 5  Optimality and run-time plots on the UCI dataset in the unconstrained setting.

Appendix D: Additional Experiments

| Dataset          | Bakery Dataset | Kosarak Dataset | Instacart Dataset |
|------------------|----------------|-----------------|-------------------|
|                  | #params | train_ll | test_ll | #params | train_ll | test_ll | #params | train_ll | test_ll |
| MNL model        | 50      | -91130   | -22889   | 2021    | -1317416 | -331857 | 5981     | -2150975 | -690322 |
| MMC model (5%)   | 62      | -77674   | -19289   | 2812    | -1389932 | -350560 | 6767     | -2722321 | -684255 |
| MMC model (10%)  | 110     | -77596   | -19303   | 3580    | -1386661 | -340553 | 9914     | -2690143 | -679505 |
| MMC model (20%)  | 292     | -77531   | -19373   | 6490    | -1379610 | -342239 | 21714    | -2624928 | -676805 |
| MMC model (50%)  | 655     | -77241   | -19411   | 12220   | -1358675 | -350582 | 45313    | -2101259 | -687172 |
| MMC model (100%) | 1261    | -76791   | -19571   | 21733   | -1325751 | -349239 | 84545    | -2346233 | -393099 |
| BundleMVL-2 model| 1261    | -76791   | -19281   | 21733   | -1325751 | -294304 | 84545    | -2346233 | -393099 |

Table 6  Log-likelihood values under different models for six additional datasets.

In Table 6, we report the fit of the BundleMVL-2 model on six additional datasets, showing that it is extremely competitive with competing models. We benchmark the performance of algorithms against the UCI dataset for: (a) the unconstrained setting in Figure 5, and (b) the constrained setting in Figure 6. Results for synthetic datasets are omitted, as they show similar trends.
For our final set of experiments, we focus on optimization using the MMC model, which is not addressed in Benson et al. (2018). We compare a MIP formulation with revenue-ordered, Adxopt and Adxopt2 in terms of run-times in Figure 7a. Next, in Figures 7b & 7c, we observe that for a fixed number of products, the time taken by Adxopt increases as the number of correction sets (H-sets) increase, while it remains unaffected for the MIP.