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Understanding Large-Scale Dynamic Purchase Behavior

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Abstract. In modern retail contexts, retailers sell products from vast product assortments to a large and heterogeneous customer base. Understanding purchase behavior in such a context is very important. Standard models cannot be used because of the high dimensionality of the data. We propose a new model that creates an efficient dimension reduction through the idea of purchase motivations. We only require customer-level purchase history data, which is ubiquitous in modern retailing. The model handles large-scale data and even works in settings with shopping trips consisting of few purchases. Essential features of our model are that it accounts for the product, customer, and time dimensions present in purchase history data; relates the relevance of motivations to customer- and shopping-trip characteristics; captures interdependencies between motivations; and achieves superior predictive performance. Estimation results from this comprehensive model provide deep insights into purchase behavior. Such insights can be used by managers to create more intuitive, better informed, and more effective marketing actions. As scalability of the model is essential for practical applicability, we develop a fast, custom-made inference algorithm based on variational inference. We illustrate the model using purchase history data from a Fortune 500 retailer involving more than 4,000 unique products.

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Keywords: dynamic purchase behavior • large-scale assortment • purchase history data • topic model • machine learning • variational inference

1. Introduction

The value of purchase history data to improve marketing activities has since long been recognized by the field (Rossi et al. 1996). An explanation for the popularity of such data are that it is one of the few data sources about revealed customer preferences that is ubiquitous. It is available at virtually any retailer. Yet, the exponential growth in assortment size in many parts of the retail landscape—especially in online retailing—has made it difficult to extract valuable managerial insights from such data. Existing methods no longer suffice.

The primary challenge in analyzing a modern retailer's purchase history data is accounting for the number and variety of products sold. On the one hand, the added value of using data to better understand customer needs and preferences increases with assortment size and diversity. Such understanding can improve marketing actions and support personalized communication. Examples are product recommendations, aiding navigation through and categorization of the assortment, and targeting activities such as personalized direct (e)mail campaigns. On the other hand, the large variety of products offered to—and

purchased by—customers makes it increasingly difficult to understand and analyze such purchase behavior.

In this article, we introduce a new model that enables marketers to gain in-depth insights from purchase history data in the context of large and varied assortments while accounting for heterogeneity across customers and shopping trips. To ensure that the model can be applied to large, realistic, retailing settings, we derive a custom-made scalable variational inference algorithm. We demonstrate the model using purchase history data from a Fortune 500 retailer that contains purchases from a large product assortment consisting of more than 4,000 products and close to 50,000 shopping trips.

Traditional applications of purchase history data have often involved fast-moving consumer goods (FMCG), for example, using scanner panel data in a supermarket (Guadagni and Little 1983, Gupta 1988, Manchanda et al. 1999). These three studies analyzed purchase behavior for only a small subset of the product assortment, considering, respectively, 8, 11, and 4 alternatives. Modern retail applications involve many more products and directly applying these methods to a large assortment is certainly not trivial,

if not impossible. In retail settings outside of the FMCG context, two additional challenges surface. First, repeat purchases of the same product either occur very infrequently or will be nonexistent for most customers. For example, consider buying products at a home improvement store, ordering products from Amazon, or watching content on Netflix. Second, often only a few products are purchased per shopping trip, both online and offline. The phenomenon of few products being purchased per shopping trip is further exacerbated by services like Amazon Prime, which guarantees free shipping with no minimum spending required. Taken together, these developments in modern retailing call for new methods to harvest the value embedded in purchase history data.

In order to accurately describe purchase behavior, any quantitative method needs to account for at least three dimensions in the data (see Manchanda et al. 1999 for a similar argument). The first two dimensions are the products and the customers, with preferences varying across customers. The third dimension relates to time, as a customer's preferences and purchase behavior may vary across shopping trips. Such preference shifts could be intrinsic to the customer, for example, because of evolving personal tastes, or driven by extrinsic contextual factors such as seasonality. These three dimensions (product, customer, and time) need to be accounted for simultaneously to properly capture the richness and complexity of purchase behavior.

Ideally, sufficient information is available to directly infer customer preferences at the product/ customer/shopping trip level. In practice, this is impossible as purchase data are very sparse across these dimensions because of several factors. First, product assortments are large and varied in modern retail environments. Second, a typical customer only purchases a very limited number of products from the complete assortment. Third, the scarce data that are available for a customer is spread out across shopping trips. The sparsity of the data, together with the size of the assortment and the need for interpretable outcomes, implies that the dimensionality of the problem needs to be reduced. This could easily be done by aggregating across products, customers, or time. However, this eliminates the ability to learn anything about the removed dimension and requires ad hoc aggregation rules, which may bias conclusions. For example, if the time dimension is ignored, seasonal products will be averaged out over time, and as a result, these products will be underexposed when they are in season.

In this paper, we introduce a model that keeps all three dimensions at the original granularity while specifying relations between products, customers, and time in a lower dimensional space. This space consists of latent dimensions that each describe a salient pattern in the purchase data. Our identification of

these dimensions is inspired by probabilistic topic models (Blei 2012), a modeling framework from the machine learning literature for text analysis. Jacobs et al. (2016) were the first to adapt this framework to purchase history data and labeled the resulting dimensions (topics) as latent *purchase motivations*. The idea is that motivations drive the observed purchase behavior in the customer base. For example, a motivation related to bathroom renovation would lead to purchases of products like PVC pipes, tiles, paint, and a bathtub, whereas a motivation related to gardening would lead to purchases of gardening supplies. The identification of such purchase motivations enables a marketing manager to reason about purchase behavior at a higher level, which can generate more insights than analyzing individual products separately, especially in the context of a large assortment.

In contrast to Jacobs et al. (2016), who aggregate over the time dimension, our model distinguishes between a customer's shopping trips to provide a more nuanced and realistic representation of purchase behavior. This enables us to generate more detailed insights for retailers. For example, at the shopping-trip level, our model can capture timerelated effects like seasonality, where some products are more relevant during a certain time of the year. The obtained insights can be even more fine grained, such as concerning the day-of-the-week or time-of-day. Dynamic, autoregressive-like dependencies across shopping trips are modeled as well, where the products bought in one trip may be informative about the products that will be purchased next. In the end, the insights generated by such a comprehensive model allow for more informed and better targeted marketing actions, connecting a customer to the relevant products, at the right time. To deal with the increased complexity of the model, we replace the inference methodology of Jacobs et al. (2016) by a custom-made variational inference algorithm that achieves computationally and statistically efficient estimates.

Industry demand for such a comprehensive and scalable method is highlighted in a research opportunity set up by Wharton Customer Analytics. In this research opportunity, a Fortune 500 specialty retailer calls for the development of tools to identify do-ityourself projects from purchase history data, where a project can be described by a collection of products. This aligns with the conceptualization of a purchase motivation. In addition, the retailer wants to be able to dynamically identify customers who are engaged in a certain project, where such engagement can potentially straddle multiple shopping trips. To foreshadow our results, the method we propose in this paper is able to identify such projects from purchase history data and to simultaneously determine the dynamics in relevance of these projects across customers and shopping trips.

The remainder of the paper is structured as follows: Section 2 introduces the conceptual and technical details of our model and positions it in the existing literature. We describe our scalable variational inference algorithm in Section 3. The data and results of our empirical application are described in Sections 4 and 5. Managerial implications are discussed in Section 6, and we wrap up with conclusions and avenues for further research in Section 7.

2. Modeling Large-Scale Purchase Behavior

In this section, we introduce our model for large-scale customer purchase behavior that builds on the topic modeling framework. To show the versatility of this framework, we start with a review of topic modeling applications in marketing. We then describe purchase motivations, that is, topics in a shopping context, at a conceptual level. After that, we introduce the formal statistical model and highlight the essential improvements compared with the LDA-X model introduced in Jacobs et al. (2016). Finally, we discuss alternative approaches to modeling dynamic purchase behavior. Throughout this section, we illustrate parts of the model using examples for a hardware store that is the context of our empirical application, but naturally our model extends to other contexts as well.

2.1. Marketing Applications of Topic Models

To develop our large-scale purchase behavior model, we build on the machine learning literature, more specifically the research on probabilistic topic models in text analysis (Blei 2012). Several articles in the recent marketing literature apply and adapt methods based on topic models, most notably latent Dirichlet allocation (LDA) (Blei et al. 2003), to provide insight in marketing problems. Most of these papers involve analyzing textual data (Tirunillai and Tellis 2014; Büschken and Allenby 2016, 2020; Puranam et al. 2017; Rutz et al. 2017; Liu and Toubia 2018), which is the traditional application of a topic model. Other papers use methods based on LDA that do not directly model text, but instead leverage the fact that LDA can model data that consists of sets of discrete outcomes.

Purchase history data were first modeled using a topic model by Jacobs et al. (2016), where purchase behavior of the customer base is described using a small set of purchase motivations (topics), and the relevance of each of these motivations is heterogeneous across customers. Our model extends this work in several ways and overcomes two of its major limitations. First, the time dimension is excluded in Jacobs et al. (2016), as the shopping trips of a customer are aggregated into a *single-basket* purchase history. This prohibits the inclusion of any time-specific effects,

identification of dynamics present in purchase behavior and shopping-trip specific idiosyncrasies. Second, the way in which customer-level heterogeneity in motivation relevance is modeled in Jacobs et al. (2016) is very restrictive, assuming all correlations between the activation of motivations to be negative. Capturing a richer correlation structure not only provides additional insights but is also particularly useful in a context with sparse information. We emphasize that lifting these limitations, while conceptually attractive, results in a large increase in the computational costs of traditional inference algorithms. We resolve this issue by developing a custom-made variational inference algorithm, outlined in Section 3.

Trusov et al. (2016) provide another application of LDA in marketing. They model website browsing behavior using an adaptation of LDA, where each household's browsing history is divided into smaller time periods. For each of these periods, the relevance over the topics is a function of both observed and unobserved heterogeneity and a lagged effect of the previous browsing period. Although the modeling approach in Trusov et al. (2016) is conceptually similar to ours, the scale of their application is several orders of magnitude smaller. They aggregate the browsing data to 29 website categories, where we consider an assortment that contains over 4,000 products in our application. Similar to us, they consider correlations between topic relevance at the customer level. However, their estimation procedure does not scale to a large number of topics, reflected by the presence of only seven topics in their application. This is in stark contrast to the 100 topics we consider in our application. The need for computationally efficient algorithms to estimate models involving large-scale data was also recently highlighted in Wedel and Kannan (2016).

Dew et al. (2020) provides another example of modeling heterogeneity using LDA. To study the evolution of product reviews, they extend LDA with a dynamic heterogeneity structure that is modeled using Gaussian processes. Although Dew et al. (2020) provide a flexible approach to capturing dynamic heterogeneity, they mention in their conclusion that their proposed method does not scale to large applications. In contrast, we introduce an inference algorithm that enables fast Bayesian inference in large retailing settings.

2.2. Connecting Topic Models to Purchase Behavior

In our model, we analyze and describe purchase behavior using a relatively small set of latent dimensions. Each of these dimensions describes a specific pattern in the purchase data. Following the nomenclature introduced in Jacobs et al. (2016), these dimensions correspond to latent *purchase motivations* that drive the observed purchase behavior in the customer base. Purchase motivations enable a marketing manager

to reason about purchase behavior at a higher abstraction level, which can generate more insights than analyzing individual products separately. Not only do these motivations shed light on relationships between products spanning different product categories, they also serve as input for marketing actions, for example, through personalization of such actions (Ansari and Mela 2003). In addition, a managerial model-based dashboard (Dew and Ansari 2018) can be constructed to help answer specific customer-behavior questions, for example, why customers visit the store during certain time periods. Targeted advertising can also be improved based on insights derived from the purchase motivations. A final example is improvements in store layout and how products are positioned relative to each other in the store, either online or offline, depending on the motivations the products are connected with.

To infer the set of purchase motivations from purchase history data, we build a new model based on the framework of probabilistic topic models (Blei et al. 2003, Blei 2012). Topic models are typically used to identify and learn about latent topics that are present in written documents. The high-level analogy between modeling text and purchase behavior is as follows: a document contains words, whereas a customer's purchase history contains products. Each word stems from a predefined vocabulary, whereas each product is purchased from a predefined assortment. A collection of documents can be summarized using a small set of topics, where each topic describes some latent theme in the text corpus; the purchase history for all customers can be summarized using a small set of motivations, where each motivation describes some preference for products. A document can be succinctly described as a mixture of topics; a customer's purchase history can be succinctly described as a mixture of purchase motivations. Such a mix of motivations enables a low-dimensional representation of a customer's preferences over the products in the assortment.

Strictly following this analogy, purchase history data would be analyzed at the customer level with the time dimension being ignored (Jacobs et al. 2016). This implies that purchases made by a customer are exchangeable across purchase trips, which is unrealistic. Variation in a customer's purchase behavior over time is to be expected and should be accounted for. For example, a customer could first visit the store for a bathroom renovation while the next trip is for pool maintenance. We capture this systematic variation by modelling a customer's purchases at each shopping trip while accounting for the interdependencies across a customer's trips.

2.3. Modeling Purchase Behavior Using Motivations

Throughout the paper we use the following notation for the data. Products are indexed by j = 1, ..., J,

where *I* is the assortment size. Customers are indexed by i = 1, ..., I, where I is the number of customers. Customer i makes B_i shopping trips. During shopping trip b customer i purchases N_{ib} products, collected in the set \mathbf{y}_{ib} . Each element in \mathbf{y}_{ib} corresponds to the index of a product: $y_{ibn} \in \{1, ..., J\}$ for $n = 1, ..., N_{ib}$. We purposefully ignore the purchase quantity of a product, as it is a measure that is difficult to meaningfully compare across different products and will (unintentionally) overemphasize products with high purchase quantities, for example, consider that only a single hammer is needed versus many nails. However, in case purchase quantity contains relevant information, the model can trivially be extended by allowing the same product to occur repeatedly in \mathbf{y}_{ih} . Characteristics that are specific to the bth shopping trip made by customer i, such as time-of-day and day-of-the-week of the trip, are captured in the K_X -dimensional vector \mathbf{x}_{ib} . Similarly, variables specific to customer *i*, like demographics or customer profile information, are captured in the K_W -dimensional vector \mathbf{w}_i .

Conceptually, purchase motivations drive—either intrinsically or by extraneous factors—the preference of a customer for a certain subset of products in the assortment. In this sense the motivation drives a customer to the store. Examples of such motivations are the plan to organize a barbecue, resulting in a preference for products related to barbecuing, or an ongoing home renovation project, resulting in a need for paint and drywall material. The underlying idea of our model is to identify a set of M purchase motivations to describe the common purchase patterns present in the customers' purchase histories (Jacobs et al. 2016). A given motivation induces the same type of purchase behavior across all customers. However, the relevance of each of the motivations naturally varies across shopping trips and customers. In practice, only very few motivations will be relevant at a single shopping trip, whereas most other motivations will not be active at all at that moment. Differences in purchase behavior across customers and shopping trips then result from variation in activated motivations.

An important feature of motivations is that they generally do not match with traditional product categorizations, like product groups or product classes. Many retailers use, or at least have used, such product categorizations, usually in the form of a product hierarchy tree. Motivations however, often span multiple product groups, as complementary products are jointly needed to achieve a goal, for example a pen and paper, or a hammer and nails. At the same time, a single product can be linked to more than one motivation. For example, working gloves can be used for gardening and for construction work.

This conceptualization of a motivation is captured in the model through a motivation-specific vector of purchase probabilities for the complete product assortment. Products that are strongly linked to the motivation will receive high purchase probabilities, whereas the other, less relevant products will have probabilities close to zero. That is, each motivation $m = 1, \ldots, M$ is characterized by ϕ_m , a J-dimensional probability vector, where $\phi_{mj} \geq 0$ denotes the probability that product j will be purchased if motivation m is activated, and $\sum_j \phi_{mj} = 1$.

Customers do not always shop with a single motivation in mind. Instead, they might go shopping for multiple motivations, for example, the kitchen and bathroom could be renovated simultaneously. The set of products a customer buys in a single trip will then be driven by a mix of motivations. The presence of multiple motivations in a single shopping trip is captured by assuming that each shopping trip is driven by a mixture of motivations. The mixture weights that govern the importance of each of the M motivations for the *b*th shopping trip of customer *i* are given by a vector $\theta_{ib} = [\theta_{ib1}, \dots, \theta_{ibM}]$, where $\theta_{ibm} \ge 0$ and $\sum_{m} \theta_{ibm} = 1$. Motivations that are irrelevant receive a weight close to zero. Variation in the motivation mixture weights across customers and shopping trips creates heterogeneity in purchase behavior.

In sum, customer i selects a purchase motivation for each purchase decision $n = 1, \ldots, N_{ib}$ in her bth shopping trip, denoted by $z_{ibn} \in \{1, \ldots, M\}$. The selection of these motivations follows the motivation mixture weights for this shopping trip—that is, the reasons for being in the store—such that

$$\Pr[z_{ibn} = m | \boldsymbol{\theta}_{ib}] = \theta_{ibm}. \tag{1}$$

Subsequently customer i buys a product based on the purchase probability vector that characterizes the motivation that drives this purchase decision, z_{ibn} . The probability that product j is purchased, given that the underlying motivation for this purchase decision is motivation m, therefore equals

$$\Pr[y_{ibn} = j \mid z_{ibn} = m, \boldsymbol{\phi}] = \phi_{mj}. \tag{2}$$

The probability vector over the assortment (ϕ_m) that is connected to a motivation is unknown to the researcher and needs to be inferred from the data. Central to the identification of these probabilities are the observed copurchases of products within shopping trips. If a certain set of products tends to be purchased together in a shopping trip, and this cooccurrence is present in many different shopping trips, then these products are likely to align with some particular motivation to shop. When motivations are active across multiple shopping trips of a specific customer, the copurchases of products across trips of this customer also help in the identification of such motivations. This is especially relevant for retail contexts

that have many shopping trips, each consisting of very few purchases.

The previous exposition connects the observed purchase behavior \mathbf{y} to the M purchase motivations. It extends the LDA-X model introduced in Jacobs et al. (2016), which only considers purchases made at the customer level and does not retain separate shopping trips. As a result, the b dimension related to the shopping trips is not present in the LDA-X model and information on the impact of shopping-trip specific variables \mathbf{x}_{ib} on purchase behavior is lost.

2.4. Modeling Activation of Purchase Motivations

With purchase motivations driving purchase behavior, the next step is to model the relevance of purchase motivations across customers and shopping trips. In the standard LDA model (Blei et al. 2003), the mixture weights θ_{ib} are draws from a Dirichlet distribution: $\theta_{ib} \sim \text{Dirichlet}(\alpha)$. However, when modeling customer purchase behavior, this has two major disadvantages.

First, the Dirichlet distribution specifies a very restrictive correlation structure. It imposes negative correlations between all pairs of motivations, and these correlations are completely determined by the mean of the distribution. This stems from the fact that the Dirichlet distribution is characterized by a single parameter vector $\boldsymbol{\alpha}$, unlike, for example, a multivariate Normal distribution that has separate parameters for its mean and covariance. This restrictive correlation structure is unlikely to reflect that of the motivation mixture weights. Some motivations are expected to be positively correlated, for example, a gardening motivation and a swimming pool motivation, whereas others might be negatively correlated.

The second drawback relates to the complexity of estimating α . If plenty of information is available, that is, if \mathbf{y}_{ib} contains many elements on average, the exact value of α is less important. Hence, in many traditional (text) applications of LDA this parameter is either fixed to some predefined value or set using heuristics (Wallach et al. 2009). In the context of purchase data, the number of products purchased in a given shopping trip is very small. Therefore, when analyzing purchases at the shopping trip level, the parameter vector of the Dirichlet distribution plays an important role and should be estimated (Jacobs et al. 2016). From a computational perspective, however, this estimation does not scale to applications that involve a large number of motivations, as the density of the Dirichlet involves a product of multiple gamma functions. This is further exacerbated when a customer-specific α_i is specified, for example as in the LDA-X model.

Instead, we opt for an alternative approach to model θ_{ib} that circumvents these drawbacks. In particular, we are inspired by the correlated topic model (CTM), which replaces the restrictive Dirichlet

distribution on θ_{ib} by a more flexible logistic Normal distribution that allows for correlations between the motivations (Blei and Lafferty 2007). To be more precise, θ_{ib} is the softmax⁵ of an unrestricted stochastic parameter vector $\boldsymbol{\alpha}_{ib} \in \mathbb{R}^{M}$:

$$\theta_{ib} \equiv \text{softmax}(\alpha_{ib}) = \frac{\exp(\alpha_{ib})}{\sum_{m} \exp(\alpha_{ibm})}.$$
 (3)

The softmax function is a natural choice here as it outputs a probability vector given any input vector of real numbers. The scalar parameter α_{ibm} can be interpreted as a measure of the (latent) relevance of motivation m in the bth shopping trip of customer i, similar to latent utilities in market share attraction models (Bronnenberg et al. 2000) or the utility-based specification of the multinomial logit model (Train 2009).

Many factors relate to the relevance of each of the M motivations in a given shopping trip. Some of these factors can be attributed to a customer's innate preferences and observed characteristics, whereas others may be driven by a shopping trip's contextual factors such as the time the trip takes place. However, after accounting for these factors, some variation in the motivation relevance remains unexplained. To account for all this, we specify a linear model for α_{ibm} that includes a predictable component μ_{ibm} , and a random, unpredictable component ε_{ibm} :

$$\alpha_{ibm} = \mu_{ibm} + \epsilon_{ibm} = \kappa_{im} + \boldsymbol{\alpha}_{ib-1}^{\mathsf{T}} \boldsymbol{\rho}_m + \mathbf{x}_{ib}^{\mathsf{T}} \boldsymbol{\beta}_m + \mathbf{w}_i^{\mathsf{T}} \boldsymbol{\gamma}_m + \epsilon_{ibm}.$$
 (4)

The customer-specific intercept κ_{im} captures the innate preferences, that is, the baseline relevance of motivation m for customer i across all shopping trips. The M intercepts for customer i are collected in the vector $\kappa_i = [\kappa_{i1}, \ldots, \kappa_{iM}]$. For κ_i we specify a multivariate Normal distribution with mean μ_{κ} and covariance Σ_{κ} . The vector μ_{κ} describes the prevalence of each of the M motivations in the customer base, while the motivation correlations are captured in Σ_{κ} .

The inclusion of these motivation correlations at the customer level is a major improvement over the commonly used Dirichlet distribution, as it enables the identification of complementarity across motivations. Knowledge of such correlations is particularly relevant for customers with only a few observed shopping trips, for whom little information is available to determine their preferences. After observing a single shopping trip, we are able to identify the most likely motivation(s) from that trip, but also the motivations that are most (cor)related to them. Let us illustrate this by foreshadowing our empirical findings: we discover multiple distinct motivations related to gardening, for example, buying plants during springtime and trash bags in fall. Intuitively, these gardening motivations are correlated at the customer

level and observing purchases in spring can be used to improve marketing actions by focusing on the correlated motivations relevant in fall.

Explanatory variables that are specific to the shopping trip, such as seasonality dummies, are included in the \mathbf{x}_{ib} vector, whereas customer-specific variables that are time invariant, for example, gender, are described in \mathbf{w}_i . Naturally the relevance of each motivation will be affected differently by these explanatory variables, and therefore the corresponding parameter vectors $\boldsymbol{\beta}_m$ and $\boldsymbol{\gamma}_m$ are motivation specific. For example, the relevance of some motivations may have strong seasonal fluctuations, whereas other motivations will hardly vary by season.

Dynamics in the model are captured by the first-order vector autoregressive, VAR(1), term $\alpha_{ib-1}^{\mathsf{T}} \rho_m$, where the relevance of each of the M motivations in the previous shopping trip directly affects the relevance of motivation m in the current shopping trip. The persistence of motivation m is described by ρ_{mm} . The cross effect of motivation m' on m, with $m' \neq m$, is described by $\rho_{mm'}$ and in general this effect is not symmetric, that is, $\rho_{mm'} \neq \rho_{m'm}$. Hence, the model contains a full $M \times M$ matrix with VAR(1)-effects. For a customer's first shopping trip, the lagged α_{ib-1} term is not available. We specify an alternative specification for μ_{i1m} , which can be found in Appendix A.

Any variation in the relevance of motivation *m* that is left after accounting for all factors mentioned previously is absorbed in the stochastic component ϵ_{ibm} . We make the following assumptions about ϵ_{ibm} . (i) Across customers, ϵ_{ibm} is independent. (ii) For a given customer, the specification of μ_{ibm} captures state dependence and variation across time. Therefore there is no autocorrelation between ϵ_{ibm} for $b = 1, ..., B_i$. iii) The relevant motivation correlations are captured by Σ_{κ} in the model. After controlling for these correlations, and given the small number of purchases per shopping trip in our application, any remaining motivation correlation at the shopping trip level can be ignored. As a result, there is no correlation across motivations ϵ_{ibm} for m = 1, ..., M. Combining these assumptions, we specify for ϵ_{ibm} a Normal distribution with zero-mean and motivation-specific variance $\sigma_{\alpha_m}^2$. This allows for heteroscedasticity, as the relevance of some motivations may be more variable than others. The model specification is completed with prior distributions for all population-level parameters, details are provided in Appendix A.

Our model nests the LDA-X model (Jacobs et al. 2016), where only the Dirichlet distribution is replaced with a logistic Normal distribution (Blei and Lafferty 2007). Specifically, LDA-X assumes the motivation mixture weights to depend only on a population-level motivation activation parameter κ_m and customer-specific

variables \mathbf{w}_i . This restricted specification results from our model specification in Equation (4) when we assume $\kappa_{im} = \kappa_m = \mu_{\kappa,m}$, $\Sigma_{\kappa} = \mathbf{0}$, $\rho_m = \mathbf{0}$, and $\beta_m = \mathbf{0}$. This shows that, apart from the distributional assumption for θ_{ib} , the LDA-X model is nested within—and a much simpler version of—our model.

2.5. Alternative Approaches to Modeling Dynamic Purchase Behavior

In the product recommendation literature, matrix factorization techniques are often used to study dependencies in preferences among large sets of products (Koren et al. 2009), and these approaches can be extended to include customer-specific characteristics (Karatzoglou et al. 2010, Baltrunas et al. 2011, Charlin et al. 2015). However, a researcher will need to decide to either aggregate over shopping trips or to treat each shopping trip independent of all other trips by the same customer. Ideas from matrix factorization are also present in dynamic factor models. Here the factorization is used inside a statistical or econometric model. For example, Bruce et al. (2012) use such methodology to study the dynamic effects of advertising on sales. However, extending such ideas to a large scale and to discrete dependent variables is not trivial.

Ruiz et al. (2020) present a probabilistic model of consumer choice that also contains matrix factorization ideas. Similar to our model, it uses purchase history data, relies on variational inference, and allows for customer heterogeneity and dependencies across products. One important difference is that it allows for product-specific characteristics such as a product's price. To model the dependencies across products, Ruiz et al. (2020) rely on the order in which products are chosen in a shopping trip. Interdependencies then arise with the current product choice depending on the products already bought in a trip.

This approach brings several challenges. First, the order of purchases is often not observed. Ruiz et al. (2020) solve this by integrating over all possible permutations using a simulation approach. Second, the dependence between products may not directly follow the sequence in time, as the order of purchases is to a large extent driven by the store layout. Ruiz et al. (2020) acknowledge this and allow the customer to *think one-step ahead*. However, this substantially adds to the complexity of the model and is only illustrated using a small-scale example in the paper. Third, our model accounts for dynamics across shopping trips, which is not possible in the approach of Ruiz et al. (2020).

Our model also differs substantially from Ruiz et al. (2020) in terms of the interpretation of the latent spaces. We build on the idea of motivations and specify probabilities for customers to have a certain motivation and for a product purchase to be driven

by a motivation. Ruiz et al. (2020) use matrix factorization inside a multinomial logit model. Their model represents products and customers as vectors in a latent space, with purchase probabilities depending on the inner products of these vectors. A customer will have maximal preference for products that appear in a certain region of the latent space. However, the dimensions of the latent space are difficult to interpret. Motivations have a direct interpretation, whereas matrix factorization requires postprocessing to facilitate interpretation.

In sum, Ruiz et al. (2020) provide a strong and useful model, especially when marketers want to intervene *during* a shopping trip. It allows for characteristics such as price and gives insights in terms of complements and substitutes. We believe that our model provides easier interpretation and is computationally more efficient. As we capture the dependence across shopping trips, it is more valuable when targeting customers who are not yet in the store.

3. Inference

The proposed model contains many latent variables and parameters that need to be estimated, we refer to this set of unknown components as Ω . The information that is available to infer Ω are the product purchases y. We apply Bayesian statistical inference and the goal is to examine the posterior distribution of Ω : $p(\Omega|\mathbf{y})$. As in most models, it is not tractable to directly evaluate this distribution. Traditionally, this problem has been circumvented by using Markov chain Monte Carlo (MCMC) methods (Rossi and Allenby 2003), in which the posterior is approximated by sampling from a Markov chain of which the stationary distribution is the posterior of interest. Asymptotically it is guaranteed that the Markov chain produces samples from the target posterior distribution. For practical purposes, however, convergence of the chain to the posterior distribution can be too slow, especially for model structures that result in complex posteriors (Carpenter et al. 2017). Given the hierarchical structure of our model and the large number of customer-specific parameters, using Hamiltonian Monte Carlo (HMC) (Neal 2011) is also ineffective. The complexity of HMC scales with the size of the parameter space, and this complexity cannot be simplified using conditional independence assumptions present in hierarchical models.

Variational inference (VI) is an alternative inference technique that is fast and scalable. VI stems from the machine learning literature and works particularly well for large-scale models (Blei et al. 2017). The general idea is to transform posterior inference into an optimization problem. The objective here is to find the distribution that best approximates the true posterior, from a prespecified class of distributions. By limiting

the class of distributions to those that are computationally convenient, one can closely approximate the posterior in a computationally efficient way (Jordan et al. 1999). Typically, the output of VI accurately describes posterior means, but underestimates posterior variances (Blei et al. 2017).

The fact that VI yields an approximation of the true posterior distribution is a theoretical disadvantage compared with the asymptotically exact sampling methods. However, there are several practical advantages that justify its use. First, convergence in VI is typically fast—much faster compared with samplingbased methods—and it is possible to monitor this convergence reliably (Ormerod and Wand 2010). Second, the output of VI is a distribution that is parameterized by a set of parameters. This is in contrast to the sampling-based methods, where for each unknown model component, a long chain of samples is needed to accurately approximate the posterior, creating a large memory burden for models with many unknown components. Third, VI can be sped up using advances from the optimization literature. Examples are stochastic subsampling, stochastic gradients, and parallelization of computations (Hoffman et al. 2013, Kucukelbir et al. 2017). These optimization techniques lend themselves well for the estimation of large hierarchical Bayesian models.

To date, VI has been adopted in few marketing papers (Braun and McAuliffe 2010, Dzyabura and Hauser 2011, Ansari et al. 2018, Xia et al. 2019, Toubia 2021). Given the scale of our application and the complexity of our model, we turn to VI as well. We derive an inference algorithm that is customized to our model structure and is computationally highly efficient. In Section 3.1, we discuss VI in general and describe our implementation of this inference technique. Compared with a straightforward application of standard VI techniques our implementation yields a better approximation to the posterior distribution, but potentially comes at a high computational cost. The need for a repeated (numerical) calculation of the inverse of a large matrix lies at the root of this. We derive an analytical solution for the inverse that completely alleviates this computational burden in Section 3.2. Section 3.3 discusses further ways to increase the computational efficiency in the context of very large data sets. In Section 3.4, we describe how to interpret the effect sizes of the explanatory variables in our model.

3.1. Estimation Using VI

In VI, the posterior inference problem is cast as an optimization problem where the search space is constructed of probability distributions. We define \mathcal{Q} as a set of joint probability distributions over the unknown model components Ω . A specific distribution—and corresponding density—is denoted by q, that is, $q(\Omega) \in \mathcal{Q}$.

We refer to q as a *variational distribution*. The objective is to find the distribution q in \mathcal{Q} that is closest to the posterior distribution $p(\Omega|\mathbf{y})$, where closeness is measured using the Kullback-Leibler (KL) divergence (Blei et al. 2017), which we denote by KL{ $q(\Omega)||p(\Omega|\mathbf{y})$ }.

In case no constraints are placed on the set \mathcal{Q} , the solution $q^*(\Omega)$ that minimizes $\mathrm{KL}\{q(\Omega)||p(\Omega|\mathbf{y})\}$ is the posterior distribution $p(\Omega|\mathbf{y})$, which cannot be evaluated directly. Instead, researchers often rely on the mean-field assumption (Bishop 2006), which states that each joint probability distribution in \mathcal{Q} factorizes over the unknown parameters Ω according to some partitioning $F(\Omega)$, with $\bigcup_{\omega \in F(\Omega)} \omega = \Omega$, such that $q(\Omega) = \prod_{\omega \in F(\Omega)} q(\omega)$. A variational distribution that minimizes $\mathrm{KL}\{q(\Omega)||p(\Omega|\mathbf{y})\}$ can then be found by using a coordinate descent algorithm that iterates over the subsets of parameters $\omega \in F(\Omega)$, updating each corresponding variational distribution $q(\omega)$ (Bishop 2006), which is guaranteed to reach at least a local optimum (Boyd and Vandenberghe 2004).

In general, by using the mean-field assumption, $\mathcal Q$ no longer contains the true posterior distribution. As a result, $q(\omega)$ should be interpreted as the variational approximation of the marginal posterior distribution of ω : $p(\omega|\mathbf{y}) = \int_{\Omega_{\setminus \omega}} p(\omega, \Omega_{\setminus \omega}|\mathbf{y}) d\Omega_{\setminus \omega}$ (Jordan et al. 1999), where $\Omega_{\setminus \omega}$ refers to all elements of Ω except ω . This does not imply that $q(\omega)$ is independent from the variational distribution for $\Omega_{\setminus \omega}$, as we are searching for the variational distribution that is closest to the complete posterior distribution $p(\Omega|\mathbf{y})$ in which the parameters depend on each other, irrespective of the partitioning $F(\Omega)$.

The partitioning $F(\Omega)$ directly controls the quality of the variational approximation. A finer partitioning is computationally easier, but also less accurate. The most fine-grained partitioning has each ω as a singleton set containing one (scalar) parameter. This implies that $q(\Omega)$ factorizes across the elements of a multivariate parameter as well, removing any posterior correlation between these elements; an unrealistic assumption in practice.

Indeed, VI has been implemented for the standard LDA model without partitioning the Dirichlet distributed parameters (Blei et al. 2003, Hoffman et al. 2013). In contrast, in the CTM model, Blei and Lafferty (2007) factorize the variational distribution for each multivariate Normal parameter into a set of independent univariate Normal distributions. This simplifying assumption facilitates estimation but reduces the quality of the variational approximation, particularly when there is substantial estimation uncertainty. In our case this is expected for the customer and shopping-trip specific parameters, as most customers tend to buy only a few products per trip. We therefore specify a partitioning $F(\Omega)$ that retains all elements of a multivariate parameter within a single

subset, ω , for *all* multivariate parameters in the model, including the customer-specific multivariate Normal parameter κ_i . Implementation details of the resulting variational inference algorithm are provided in Appendix B.

3.2. Computational Efficiency

The partitioning $F(\Omega)$ in our implementation of variational inference is guaranteed to improve the quality of the variational solution but is computationally costly. Specifically, it involves the optimization of many multivariate Normal variational distributions. For example, each κ_i has a customer-specific variational distribution $q(\kappa_i) = \text{MVN}(\tilde{\mu}_i, \tilde{\Sigma}_i)$. Determining the optimal value for $\tilde{\Sigma}_i$ in each iteration of the optimization routine involves computing the inverse of an $M \times M$ matrix that is specific to customer i of the following form (cf. Equation (B.9)):

$$\tilde{\Sigma}_i = (\tilde{E}\{\Lambda_{\kappa}\} + d(\tilde{E}\{\tau_{\alpha}\})s_i)^{-1}, \tag{5}$$

where s_i is a customer-specific scalar, $\Lambda_{\kappa} \equiv \Sigma_{\kappa}^{-1}$, and $\tau_{\alpha} \equiv [\sigma_{\alpha_1}^{-2}, \dots, \sigma_{\alpha_M}^{-2}]$. The operator \tilde{E} denotes an expectation under the marginal variational distribution for a parameter, for example, $\tilde{E}\{\Lambda_{\kappa}\}\equiv E_{q(\Lambda_{\kappa})}\{\Lambda_{\kappa}\}$, and d() is a function that outputs a diagonal matrix based on an input vector.

Therefore, in a naive implementation, each iteration of the optimization algorithm has a computational complexity of at least $\mathcal{O}(I \times M^3)$, which clearly does not scale well with the number of customers I nor the number of motivations M. As a result, our improved partitioning would render this approach computationally infeasible in large applications of the model.

We completely remove this computational burden by exploiting a special mathematical structure in the optimal value for $\tilde{\Sigma}_i$. Note that $\tilde{\mathbb{E}}\{\Lambda_\kappa\}$ and $d(\tilde{\mathbb{E}}\{\tau_\alpha\})$ are nonsingular precision matrices that are specified at the population level and, hence, shared between all customers $i=1,\ldots,I$. The only customer-specific part is s_i , the scaling factor for $d(\tilde{\mathbb{E}}\{\tau_\alpha\})$. Our computational shortcut is obtained from the fact that $\tilde{\Sigma}_i$ can be rewritten as

$$\tilde{\Sigma}_i = (\mathbf{L}^{-1})^{\mathsf{T}} \mathbf{U} d((\mathbf{v} + s_i)^{-1}) \mathbf{U}^{\mathsf{T}} \mathbf{L}^{-1}, \tag{6}$$

where **L** is the lower triangular Cholesky root of $d(\tilde{E}\{\tau_{\alpha}\})$ —which for a diagonal matrix is equivalent to the square root of its diagonal elements—and $\mathbf{U}d(\mathbf{v})\mathbf{U}^{\mathsf{T}}$ is the singular value decomposition of $\mathbf{L}^{-1}\tilde{E}\{\mathbf{\Lambda}_{\kappa}\}(\mathbf{L}^{-1})^{\mathsf{T}}$. Appendix C provides a proof of this result. This equivalence shows that $\tilde{\Sigma}_i$ can be computed for any customer i without directly taking the inverse of a customer-specific $M \times M$ matrix. Similar results can be obtained for the covariance matrices of $q(\rho_m)$, $q(\beta_m)$,

and $q(\gamma_m)$. This result enables us to obtain a better approximation for the posterior distribution, without incurring insurmountable computational costs when many customers and motivations are involved. This result is also an addition to the variational inference literature and can directly be applied to other hierarchical models involving multivariate Normals, such as the CTM.

3.3. Scalability of the Inference Algorithm to Very Large Data Sets

Because of the efficient matrix inverse identity presented in Section 3.2, the vast majority of the computation time of our inference algorithm is spent on the update of the variational distributions that are specific to a product purchase or a shopping trip, that is, z_{ibn} and α_{ib} . For a given number of motivations M, the computation time of a single iteration scales linearly with the number of shopping trips and purchases. In other words, if a large data set doubles in size, the required computational time will approximately double as well.

However, because the customers are conditionally independent in the model, there are multiple ways to improve scalability. First, the customer-specific optimizations can be parallelized over the customers, so the available computing power can be easily increased by using a computing cluster. Second, stochastic optimization techniques can be used (Hoffman et al. 2013), which reduce the number of epochs needed to achieve convergence, especially for large data sets. This lets our inference algorithm scale to data sets of virtually any size, which is an important advantage of estimation using variational inference. Even without such extensions, the required computational time of our model is relatively low. For the empirical application in this paper, estimation is completed in a matter of hours on a standard laptop. In this time, we complete 1,000 iterations of the algorithm for M = 100, whereas model convergence was already achieved within the first few hundred iterations.

3.4. Quantifying the Effects of Explanatory Variables

Our model contains several explanatory variables—both latent (α_{ib-1}) and observed $(\mathbf{x}_{ib}, \mathbf{w}_i)$ —that affect the relevance of motivations at the shopping-trip level. To interpret the model results, the effect sizes of these explanatory variables should be judged. The corresponding coefficients $(\rho_m, \beta_m, \gamma_m)$, could be evaluated directly to learn about the linear effects of the explanatory variables on the relevance of motivation m: α_{ibm} . However, motivation relevance is an abstract latent construct that is not straightforward to interpret. A more tangible model component is the vector of

motivation-activation probabilities θ_{ib} , defined as the softmax of α_{ib} (cf. Equation (3)). Understanding how these probabilities are affected by the explanatory variables enables us to answer managerially relevant questions such as: "How does gender affect motivation activation?" or "How does time of the day shift the likelihood of various motivations?". To this end we calculate odds ratios for the motivation-activation probabilities, where we contrast the motivation probabilities corresponding to a certain value of the characteristics to those of the average shopping trip.

Because θ_{ibm} is a nonlinear function of α_{ib} , the effect of a focal explanatory variable depends on μ_{ibm} = $\kappa_{im} + \alpha_{ib-1}^{\top} \rho_m + \mathbf{x}_{ib}^{\top} \boldsymbol{\beta}_m + \mathbf{w}_i^{\top} \boldsymbol{\gamma}_m$ and the disturbance term ϵ_{ib} (cf. Equation (4)). Hence, to provide an interpretation to the effect of a focal explanatory variable, sensible baseline values for all explanatory variables need to be specified and integration over the distribution of ϵ_{ib} is needed. We use the average shopping trip as a natural baseline. For this baseline, we set the exogenous explanatory variables \mathbf{x}_{ib} and \mathbf{w}_i to their sample means, the motivation intercepts in κ_i to their population-level mean (μ_{κ}) , and the lagged α_{ib-1} to the average posterior mean over all α_{ib} . We use the posterior means for the population-level parameters, as the information available for those parameters is large, and therefore their posterior variance is small. Together, this set of baseline values is used to compute μ^B .

Next, we consider a particular characteristic and, ceteris paribus, change its value relative to the baseline. For a continuous characteristic we consider a shock relative to its baseline value, whereas for a discrete characteristic, we simply consider a particular level and set the explanatory variables accordingly. These shifted values are used to compute μ^S .

The odds ratio of a characteristic is then defined by taking the ratio of the probability of motivation m after the corresponding shift in variables (θ_m^S) and the baseline probability (θ_m^B) , while integrating out the disturbance, that is,

$$E\left\{\frac{\theta_{m}^{S}}{\theta_{m}^{B}}\right\} = \int_{\varepsilon} \frac{\exp(\mu_{m}^{S} + \varepsilon_{m}) / \sum_{\ell=1}^{M} \exp(\mu_{\ell}^{S} + \varepsilon_{\ell})}{\exp(\mu_{m}^{B} + \varepsilon_{m}) / \sum_{\ell=1}^{M} \exp(\mu_{\ell}^{B} + \varepsilon_{\ell})} \times p(\varepsilon) d\varepsilon, \tag{7}$$

where $p(\varepsilon)$ denotes the density of ε , that is, $\varepsilon_m \sim N(0, \sigma_{\alpha_m}^2)$ for m = 1, ..., M. This odds ratio can be computed for—and is comparable across—all characteristics, as the baseline μ^B is the same for each.

4. Data

We apply our model to in-store purchase history data recorded at the shopping-trip level that is made available to us by a Fortune 500 Specialty Retailer.⁸ The data contain purchases made by customers in one of their retail stores in Florida during a 24-month period that ranges from March 5, 2012 to March 4, 2014. Customers are known to the retailer, such that different shopping trips can be linked to the same customer. In addition to purchase behavior some information on customer demographics is available, including age, gender, and household size. Descriptive statistics for these variables are presented in the online appendix.

The raw data contain information on purchase incidence for 29,027 distinct products by 2,259 distinct customers. Most of these products are purchased very infrequently: 25,726 products are purchased in less than 10 shopping trips during the 24-month time span. In principle, our model works for very infrequent products as well. However, we are interested in gaining substantive insights from the data instead of capturing purchase patterns that are driven by just a few co-occurrences between infrequently purchased products. Instead of removing the infrequently purchased products from the data altogether, we aggregate the infrequent products according to the firm's product taxonomy.

The product taxonomy defines a product as a unique combination of [Group, Class, Subclass, Description]. For example, a product in the data are [Group = BUILDING MATERIALS, Class = GYP-SUM, Subclass = BOARD, Description = "1/2" X4'X8' USG MOLDTOUGH DRYWALL"]. Another product within the same [Group, Class, Subclass] combination but with a (slightly) different description such as "1/ 2"X4'X8' USG ULTRALIGHT DRYWALL" is considered to be a different product in the data. Products that are purchased very infrequently are aggregated according to this product taxonomy as follows. For each [Group, Class, Subclass] combination, the corresponding infrequent products are merged. If the aggregate product is still infrequently purchased, the same step is repeated for each [Group, Class] combination and, if necessary, subsequently at the [Group] level. At the end of this aggregation process, only 19 infrequent products remain that are purchased less than 10 times, corresponding to 34 purchases in the data. These products have been removed from the data.

The resulting data set contains 139,622 purchases out of an assortment of 4,266 distinct products. The purchases are made by 2,259 unique customers across 47,568 shopping trips. Some descriptive statistics of the purchase data are displayed in Table 1. The statistics illustrate a loyal customer base, with on average 21.06 shopping trips per customer. However, the amount of information per shopping trip is small. The average number of products purchased per shopping trip is only 2.94, and on average, a product in the assortment is purchased in 32.73 shopping trips.

	Mean	Mode	Min	25%	Median	75%	Max
Purchases per trip	2.94	1	1	1	2	4	50
Purchases per product	32.73	10	10	12	18	31	724
Trips per customer	21.06	1	1	8	16	28	257
Purchases per customer	61.81	1	1	21	46	85	645

Table 1. Descriptive Statistics of the Purchase History Data

Such figures are representative for other modern retailing environments, where the cost of holding a large product assortment is low, and customers are encouraged to place many small orders with low shipping costs, for example, consider the subscription service Amazon Prime. At the product level the data are sparse, with more than half of the products being purchased less than 20 times across the almost 50,000 shopping trips.

We split the data set in two parts: an in-sample part—used to estimate the model parameters—and an out-of-sample part—used to determine the model's predictive performance. As out-of-sample data we take the last shopping trip for every customer that has visited the store more than once. Characteristics of the different data sets are displayed in Table 2.

5. Results

This section is organized as follows. We first describe some high-level characteristics of the inferred set of purchase motivations in Section 5.1. Using these motivations, we describe and visualize the customer journey for two customers in Section 5.2. In Section 5.3, we enrich our understanding of the motivations by examining how the relevance of motivations is affected by both the timing of the trip and customer characteristics. The relations between motivations based on the correlations and VAR(1)-effects are discussed in Section 5.4. We conclude in Section 5.5 by comparing the predictive performance of our model against several benchmarks.

The results in this section are based on the inferred variational posterior distribution of the model parameters. Generally, closed-form expressions do not exist for expectations of nonlinear functions of parameters under the posterior distribution. As an abundance of information is available for the population-level parameters, and hence very little posterior uncertainty, we use the posterior mean value when evaluating functions that involve these parameters. In contrast,

Table 2. Characteristics of the Different Sets of Purchase History Data

	Products	Customers	Trips	Purchases
Complete	4,266	2,259	47,568	139,622
Estimation	4,266	2,259	45,473	134,049
Out-of-sample	2,396	2,095	2,095	5,573

for parameters that relate to either a shopping trip or a customer, much less information is available, and we rely on Monte Carlo integration with 250,000 samples to account for the posterior uncertainty.

5.1. Purchase Motivations

Based on the large number of customers, products, and shopping trips, we expect substantial heterogeneity in purchase behavior. In the model we can account for this by setting the number of purchase motivations, M, to a large value. At the same time, we are interested in gaining substantive insights from the data, that is, identifying motivations that are relevant from both a managerial and a customer perspective. This implies that M should also not be too large.

One approach to determine *M* is to use some performance measure, for example, predictive performance on holdout data. However, this does not factor in interpretability of the model and one could end up with too many motivations for the model to be of practical use. Instead we set M = 100. We anticipate that this configuration allows us to identify the salient purchase patterns in the data, as well as more specific patterns that may only be relevant for a small subset of the shopping trips or customers. Furthermore, Jacobs et al. (2016) have shown that specifying a value for Mthat exceeds the actual number of motivations does not significantly impede predictive performance, as long as the proportions for the motivations are estimated at the population level, which is the case for our model. In addition, the ability to deal with such a large number of latent motivations also demonstrates the scalability of our model.

The size of each of the m = 1, ..., M purchase motivations is displayed in Figure 1, which reports the expected number of purchases for each motivation under the posterior distribution. The motivations are sorted in descending order of size, which ranges from 4,021.36 purchases (3.00%) for m = 1 to 717.48 purchases (0.54%) for m = 100. This shows that there is variety in motivation size and that all motivations are relevant.

Each motivation m is characterized by ϕ_m , a vector of purchase probabilities for all products in the assortment. For a motivation to be managerially useful, it should relate to a clear and relatively small subset of the assortment; that is, ϕ_m should be a sparse

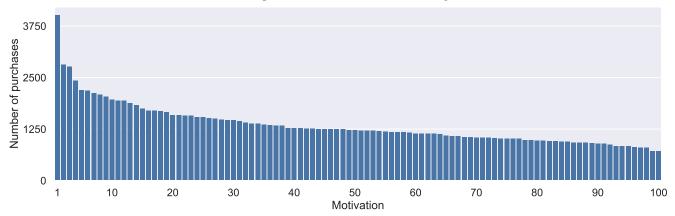


Figure 1. (Color online) Size of Motivations (Expected Number of Purchases Assigned to Each Motivation)

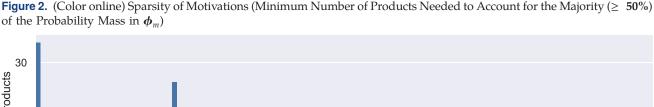
probability vector with many values close to zero and a limited number of large purchase probabilities. Figure 2 shows, for each motivation *m*, the minimum number of distinct products needed to account for at least 50% of the product purchases under that motivation. The vast majority of the motivations is very sparse as more than half of their product purchases are covered by fewer than 10 products, which is a very small fraction of the 4,266 products in the whole assortment. The largest motivation identified (m = 1) is also the motivation that is least sparse. Intuitively this makes sense, as a broad motivation is more likely to appeal to a large part of the customer base.

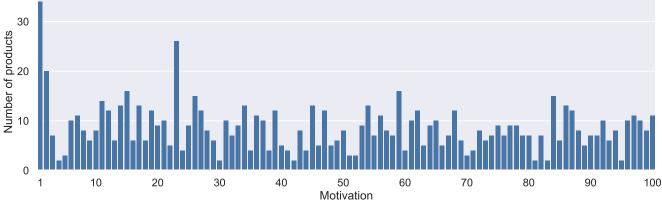
Motivations are characterized by the products that are most likely under that particular motivation. The larger the cumulative probability of these products, the better they summarize the whole motivation. However, summarizing and labelling a motivation is subjective. An expert's opinion, such as that of a product manager at the retailer, will facilitate this task. In absence of such an expert we rely on the available product taxonomy and introspection for labeling the *M* motivations. We emphasize that the

product taxonomy is not used in the model to identify the motivations but is solely used to facilitate interpretation of the model output.

Table 3 presents the labels we assigned to the 10 largest motivations based on the most likely products for each motivation. It also shows the cumulative purchase probability covered by the 10 most likely products under each motivation, which varies substantially across motivations. For the largest motivation, it is 23.42%, again indicating that this is a broad motivation with probability mass allocated to a relatively large number of products. On the other hand, for the fourth largest motivation, the cumulative purchase probability for the 10 most likely products purchased under that motivation is 84.69%, so these 10 products almost completely describe this motivation.

An important message from this paper is that marketers should use motivations instead of-or at least besides—existing product categories, because customer purchase behavior spans across multiple product categories. To illustrate this, we display the 10 most likely products with information from the





product taxonomy for motivation 12 in Table 4 and motivation 6 in Table 5. Motivation 12 is related to doit-yourself projects concerning deck and fence installations. Motivation 6 leads to purchases of wall plates, that is, the installation of light switches and power outlets. Table 4 shows that the 10 most likely products for motivation 12 are spread out across three groups, six classes, and eight subclasses. This motivation is an example of a purchase pattern that clearly covers products from multiple product categories. Table 5 for motivation 6, on the other hand, tells a different story: the 10 most likely products are contained in a single group and two classes, although still spread out over five different subclasses. Hence, this purchase pattern is more in line with the existing product taxonomy. Our modeling approach has the flexibility to capture both scenarios.

Some of the motivations highlight products that are not very frequently purchased, whereas other motivations are of course driven by high volume products. To illustrate this, we consider the purchase-frequency ranks of the most likely products under each motivation. The product with rank = 1 has the highest purchase volume in the data, which is a bag of fasteners (e.g., screws, nuts, bolts). It is the most likely a product under motivation 4, which indeed relates to fastener products. More interestingly, motivation 23, which relates to exterior paint jobs and waterproofing, places the highest purchase probability on an exterior paint product, which only has a rank of 588 in the data. Descriptive statistics of the ranks for the five most likely products under each motivation are given in Table 6. For the most likely product, the average rank of 116.49 indicates that other motivations also highlight products that are relatively infrequently purchased. If we look beyond the single most likely product under each motivation, we notice that even more products in the tail of the assortment are identified as highly relevant for a motivation. This shows that by using the motivations, our model is able to highlight purchase patterns that also involve low-volume products.

Another advantage of our method is that it results in soft clusters of products, that is, the same product can be relevant for more than one purchase motivation. For example, we identified several motivations related to plumbing, each involving pipes of different widths. For each of these motivations the "1/2"X260" PTFE THRD SEAL TAPE" (PTFE Thread Seal Tape) product receives a relatively high purchase probability, which intuitively makes sense as it is needed in different plumbing projects. In a hard clustering approach, this product could only have been assigned to a single motivation. Similar examples in our empirical application are identified for multiuse products such as paint brushes, caulks, and cement mixes.

5.2. Customer Journey

A customer's journey at the retailer can be succinctly described and visualized using the identified motivations. In Figures 3 and 4, we illustrate the journey for two customers at the retailer that each have made 10 shopping trips. For each shopping trip, the motivation-activation probabilities are displayed as a set of line plots, where we focus on motivations that have a substantial probability in at least one of the shopping trips for a customer. From these figures, several distinct patterns can be identified.

Customer 144 in Figure 3 is primarily interested in gardening activities, combined with a do it yourself (DIY) project related to kitchen renovation. The kitchen renovation motivation is only active for three purchase trips in a row in June 2013. In contrast, the gardening motivations are more persistent across the shopping trips.

Similarly, customer 211 in Figure 4 is interested in gardening as well, but has different needs compared with customer 144. This is reflected by the activation

Table 3. Labels for the 10 Largest Motivations with the Cumulative Purchase Probability of the 10 Most Likely Products Under Each Motivation

m	Label	Cumulative probability for top 10		
1	Painting: Paint tools and supplies	23.42%		
2	Cleaning: General cleaning supplies	38.78%		
3	Gardening: Annuals and perennials	59.63%		
4	Hardware: Fasteners (screws, nuts, bolts, washers)	84.69%		
5	Gardening: Landscaping (mulch and top soils)	87.87%		
6	DIY: Wall plates	50.88%		
7	DIY: Electrical installations	48.73%		
8	DIY: Tile installation	59.43%		
9	Gardening: Seeds, vegetables, herbs	66.56%		
10	Cleaning: Floors	56.48%		

Table 4. Ten Most Likely Products (Cumulative Probability, 45.15%) for m = 12 (DIY: Deck and Fence Installation)

Probability	ability Group Class		Subclass	Description		
7.30	Lumber	Pressure trtd wood	PT dimensional lumber	2x4-8ft #2 prime pt weathershield		
6.37	Building materials	Metal products	Metal prod/simpson	_		
4.93	Hardware	Fasteners	Deck screws	_		
4.88	Hardware	Builder's hardware	Gate hardware	_		
4.47	Lumber	Fencing	Pressure treated pickets	5/8"x5-1/2"x6' pt pine dog ear pckt		
4.32	Lumber	Pressure trtd wood	PT timbers	4x4-8ft #2 pt		
3.55	Lumber	Pressure trtd wood	PT dimensional lumber	2x4-8ft #2 pt		
3.44	Building materials	Concrete	Concrete mixes	50lb sakrete fast-set concrete		
3.01	Hardware	Fasteners	Construction/frming nail	_		
2.88	Lumber	Pressure trtd wood	PT dimensional lumber	_		

Note. Missing information in the product taxonomy, for example, a description for an aggregated product, is indicated by -.

of different gardening motivations. Customer 211 seems to be more focused on landscaping and is not interested in DIY projects. On the other hand, motivations related to Christmas, cleaning, and rust preventative spray paints are relevant to this customer as well.

The journeys of these two customers also highlight the necessity for modeling purchase behavior at the shopping trip level instead of the customer level. Each customer could be described by some general customer profile, or a mix of those, for example a *gardener* or a *do-it-yourselfer*. However, within these profiles, there is substantial variation across shopping trips and between customers. By modeling purchase behavior at the shopping trip level, we are able to capture this variation, which in turn enables us to find more nuanced motivations that describe a customer's profile more accurately.

5.3. Effects of Explanatory Variables

The relevance of motivation m in shopping trip b of customer i is, among other things, a function of explanatory variables specific to the shopping trip, \mathbf{x}_{ib} , and the observed customer characteristics, \mathbf{w}_i . In our application, the variables in \mathbf{x}_{ib} relate to the timing of the trip, for example, month, weekday versus weekend, daytime versus evening. The available customer characteristics \mathbf{w}_i are age brackets, gender, and a proxy for

household size. For these explanatory variables, we measure the effect on motivation relevance by considering odds ratios as defined in Section 3.4, where the baseline is the average shopping trip. We report descriptive statistics across the different motivations for the odds ratios related to all variables in \mathbf{x}_{ib} and \mathbf{w}_i in the online appendix.

The descriptive statistics show that the shoppingtrip specific variables \mathbf{x}_{ib} have substantial effects on motivation relevance and that these effects vary across motivations. We illustrate this with some examples: the weekend dummy increases the likelihood for motivation 72 by 26.6% (odds ratio, 1.266). Further inspection shows that this motivation relates to grills and patio furniture. On the other hand, motivation 42, which is about key and lock replacements, becomes 17.8% less likely during the weekend (odds ratio, 0.822). At the same time, this motivation has a large positive shift of 23.9% for shopping trips after work hours, which seems intuitively plausible. The largest odds ratios are obtained for November (29.449) and December (34.194), both for motivation 20. These extreme odds ratios make sense, as motivation 20 is about Christmas and holiday decorations.

A similar analysis can be made for the customer characteristics in \mathbf{w}_i . Again, we see a substantial spread

Table 5. Ten Most Likely Products (Cumulative Probability, 50.88%) for m = 6 (DIY: Wall Plates)

Probability	Group	Class	Subclass	Description
11.58	Electrical	Wiring devices	Wall plates (commodity)	_
10.02	Electrical	Wiring devices	Receptacles	_
7.65	Electrical	Wiring devices	Switches	_
6.32	Electrical	Wiring devices	Wall plates (decorative)	_
3.89	Electrical	Wiring devices	Wall plates (commodity)	1g wht nyl midway outlet wallplt
2.66	Electrical	Wiring devices	Wall plates (commodity)	1g wht duplex wallplt
2.47	Electrical	Wiring devices	Wall plates (commodity)	1g wht decora wallplt
2.38	Electrical	Wiring devices	Wall plates (commodity)	1g wht nyl midway decora wallplt
2.15	Electrical	Wiring devices	Switches	20/10a nkl decor on/offsp tggl swtch
1.76	Electrical	Conduit/boxes/fittings	PVC box/covers/access	Old work 1g 14cu

Note. Missing information in the product taxonomy, for example, a description for an aggregated product, is indicated by -.

	Mean	Min	25%	Median	75%	Max
Rank of most likely product	116.49	1	31	78	166	588
Rank of second most likely product	206.03	3	78	177	277	626
Rank of third most likely product	296.56	4	156	277	382	755
Rank of fourth most likely product	413.28	61	235	382	571	1,128
Rank of fifth most likely product	528.71	25	301	464	713	1.676

Table 6. Descriptive Statistics of the Purchase-Frequency Rank of the Five Most Likely Products Under Each Motivation

Note. The statistics are computed across the *M* motivations.

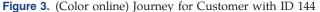
of effect sizes for the different characteristics, indicating that demographics are informative of motivation relevance. For example, for customers that are 65 years or older, the largest positive shift in motivation relevance is a 74.7% increase for a gardening motivation that involves fertilizers and flower care (m = 59). An interesting find is that large odds ratios are obtained for the dummy variables that correspond to missing values for a customer's age and gender. This shows that customers who do not provide this information, differ a lot from those who do.

In Figure 5, we zoom in on the odds ratios corresponding to a specific customer characteristic. The odds ratios for the male dummy variable show that some of the technical motivations related to DIY and plumbing are more relevant for males. This approach of finding (ir)relevant motivations for a given characteristic can be applied to all explanatory variables. In the same vein the model results could be used to determine the likely motivations for a specific demographic profile, for example, female customers in the age of 35–45 living in a large household. Such data-driven insights can be useful to further understand the customer base and to help better target specific groups of customers. In addition, the demographic

profile could be extended by considering a particular time frame, for example, a weekend in October. These modelbased odds ratios can be integrated into model-based dashboards that support marketing managers in identifying relevant motivations for targeted customer segments.

Up to this point we have provided interpretations from the perspective of the explanatory variables describing a customer and shopping trip in order to identify the most relevant motivations. Turning this idea around makes a motivation the unit of analysis. This supports managers in identifying the likely demographics and time periods for a motivation of interest. There are two advantages to this approach. First, this enables marketers to identify the segments in the customer base for which the focal motivation is relevant and to identify the time period during which its relevance peaks. Second, the explanatory variables can aid in the task of describing and interpreting a motivation, in addition to the most likely products for a motivation. This is especially useful when no detailed product taxonomy is available.

In Figure 6, we display the odds ratios of a set of explanatory variables for four selected motivations. Motivation 16 in Figure 6(a) is about food products, like sodas and snacks. We observe a large positive



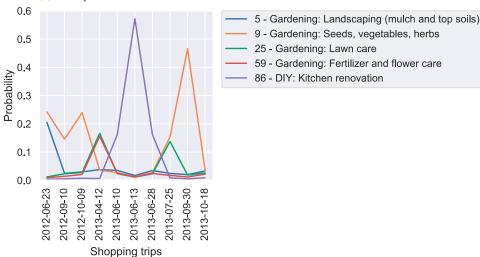
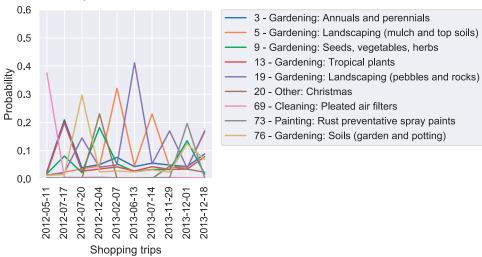


Figure 4. (Color online) Journey for Customer with ID 211



shift for this motivation for shopping trips that take place during the evening and for younger customers. Motivation 72 is about grills and patio furniture and has a strong seasonality component where the motivation is more likely in July and during weekend shopping trips (Figure 6(b)). Motivations 29 and 34 in Figure 6, (c) and (d), both relate to gardening. The seasonality patterns, however, are different. Motivation 29 is about soils and mulch, and this motivation is more likely in the period from March to May and for older customers. On the other hand, motivation 34, which is about landscaping equipment such as trimmers, mowers, and chainsaws, is more likely later in the year from June to September. This shows that even if one would have identified that a customer is interested in gardening, the relevance of specific motivations related to gardening is different across time and individuals. In contrast, if our model for purchase behavior would have aggregated shopping trips to the customer level, these separate motivations would have been aggregated into a single overarching gardening motivation, and as a result,

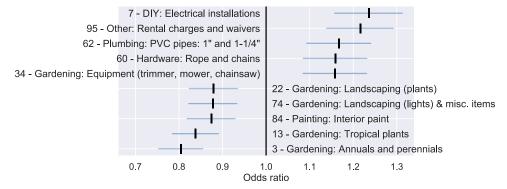
these seasonality effects would have been lost. By accounting for dynamics in shopping behavior, that is, by not aggregating across the shopping trips of a customer in the model, we have enabled the identification of such subgoals within a broader motivation such as gardening.

5.4. Relations Between Motivations

The model captures correlations across the relevance of motivations at the customer level through Σ_{κ} with corresponding correlation matrix $Corr(\Sigma_{\kappa})$. Not only do these correlations lead to better predictive distributions (Blei and Lafferty 2007), they also provide additional insight in the relations between motivations. Such insights can help identify cross-selling opportunities or assist in targeting customers that have not yet engaged in a motivation that is likely for them, based on their activities in (cor)related motivations.

The results reveal strong positive correlations of up to 0.844 for a pair of motivations that are both related to gardening (m = 3 and m = 29). The most negative correlation is -0.758 between motivation 29 and

Figure 5. (Color online) Odds Ratios Corresponding to the Gender: Male Customer Characteristic



Note. The posterior mean and 95% highest posterior density interval are displayed for the motivations with the five largest and five smallest odds ratios for this variable.

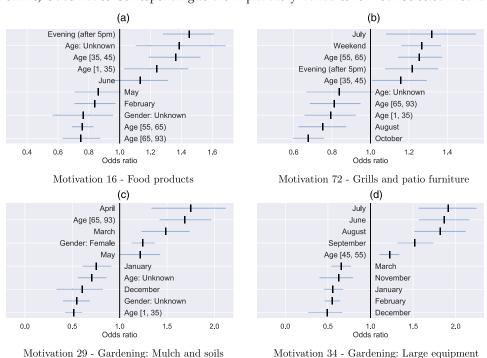


Figure 6. (Color online) Odds Ratios Corresponding to the Explanatory Variables for Four Selected Motivations

Note. The posterior mean and 95% highest posterior density interval are displayed for the five largest and five smallest odds ratios.

motivation 39, which is about drywall materials. A sizable portion of the correlations is relatively large; for example, about 3.1% of the pairwise correlations exceeds 0.50 and about 3.3% falls below -0.50. This shows that substantial correlations exist between the motivations.

To interpret the correlation structure among motivations, one can zoom in on a focal motivation and analyze which motivations correlate with that motivation. As an example, Table 7 lists the motivations that correlate most strongly with motivation 47, which is about concrete mixes. Again, the results show interesting insights that have high face validity. A motivation for concrete mixes positively correlates with certain DIY projects and hardware but negatively correlates with motivations related to cleaning products.

Table 7. Most Extreme Correlations for Motivation 47 (Concrete Mixes)

m	Motivation label	Correlation
12	DIY: Deck and fence installation	0.579
11	DIY: Lumber (studs, strips, sheathing)	0.564
37	Plumbing: PVC pipes: 1-1/2" and 2"	0.559
:	:	:
46	Cleaning: Chemicals	-0.424
10	Cleaning: Floors	-0.428
2	Cleaning: General cleaning supplies	-0.538

The previous analysis examines a one-to-many relationship for each motivation in isolation. An alternative approach is to directly visualize the relationships between all M motivations as captured by the correlation matrix. Multidimensional scaling (MDS) is a technique that maps objects to a lower-dimensional space based on their pairwise dissimilarities. The correlation matrix corresponding to Σ_{κ} can be converted to an $M \times M$ dissimilarity matrix D with elements: $D_{mm'} = \sqrt{2 - 2 \text{Corr}(\Sigma_{\kappa})_{mm'}}$ (Borg and Groenen 2005). With dissimilarity defined in this way, motivations that have a strong positive correlation will be placed close together in the MDS space, whereas motivations with small or negative correlations will be positioned further apart.

Figure 7 displays a two-dimensional MDS solution based on the dissimilarity matrix *D*. Most of the motivations can be roughly categorized in broad overarching themes such as Gardening, Plumbing, or Painting. Each of the six subfigures in Figure 7 accentuates such a theme. This reveals that most of the themes are concentrated in different regions in the graph, suggesting positive correlations between the corresponding motivations. For example, the gardening motivations can be found at the top left of the MDS plot (Figure 7(a)), whereas the south/southeast covers the more technical DIY projects (Figure 7(b)), for example, those that involve electrical installations, drywalls, and woodworking.

(a) Gardening DIY projects (c) (d) Plumbing Cleaning Painting Hardware

Figure 7. (Color online) Two-Dimensional MDS Solution Based on the Motivation Correlation Matrix $Corr(\Sigma_{\kappa})$

 $\it Note.$ Each subplot accentuates a different group of motivations from the same MDS solution.

Plumbing and Hardware overlap in location with the DIY projects. This could be expected, as plumbing can be seen as a special case of a DIY project, and hardware is needed to complete a DIY project. The two DIY motivations that are close to the gardening space are about the installation of an irrigation

1.20

9

1.10

1.05

Motivation

Figure 8. (Color online) Posterior Means and 95% Highest Posterior Density Interval for the Odds Ratios of the *Own* AR Effects of the Motivations

sprinkler system (m = 21) and the installation of screens and rodent control measures (m = 67). Indeed, such activities are expected to be related to gardening. The outlying DIY project (m = 79) relates to small bathroom repairs to the sink, drain, or toilet. Such a small-scale project is indeed less similar to the other more involved and technical DIY projects.

10

An interesting result is shown in Figure 7(e) for the motivations related to painting. All but one of these motivations are placed close together. Inspecting the outlying motivation 23 more closely reveals that it is a paint motivation dealing with exterior painting and waterproofing structures. Such a project differs in many aspects from an ordinary paint job like painting an indoor wall, explaining its distinctive position.

In summary, if one has a particular motivation in mind, it can suffice to analyze the motivations that strongly correlate with that motivation. On the other hand, if one is interested in gaining insights about groups of motivations and how these relate, a visualization method such as MDS can be more appropriate as it reduces the high-dimensionality of the pairwise correlations to an interpretable graphical representation. The common denominator is that these results have high face validity and are mostly according to intuition. Even in case the position of a motivation is surprising at first, it typically can be placed in context by examining the motivation in more detail, as we have illustrated previously. However, this does not mean that one would be able to identify and quantify these relations without the aid of our model.

In addition to the covariance matrix Σ_{κ} , relations between motivations are modeled by the VAR(1)-effects in the specification of motivation relevance α_{ib} . The VAR(1)-coefficient vector ρ_m gives the effect of the lagged motivation relevance vector (α_{ib-1}) on the relevance of motivation m: α_{ibm} . Similar to the coefficients for the other explanatory variables, the impact of the VAR(1)-coefficients can be assessed using the odds ratio as defined in Equation (7). The effect for a single lagged motivation m on the odds ratios of all M motivation activation probabilities is measured by increasing the lagged relevance of m

 $(\alpha_{i,b-1,m})$ by two standard deviations $(2\sigma_{\alpha_m})$, ceteris paribus. We can split the resulting odds ratios in an *own* autoregressive (AR) effect, for motivation m on itself, and cross AR effects, for motivation m on the other M-1 motivations.

The posterior mean and 95% highest posterior density interval for each own AR effect is displayed in Figure 8. The posterior means range from 1.019 to 1.186, with an average of 1.057. Each of these effects is larger than 1, indicating at least some persistence for all motivations. A number of motivations have a relatively large own AR effect. Examples are motivation 1 (effect 1.186), related to painting supplies, motivation 8 (effect 1.175), related to tile setting, and motivation 7 (effect 1.144), which is related to electrical installations. These motivations seem to correspond to large or persistent projects, as they are more likely to be activated across consecutive shopping trips. Other motivations have smaller own AR effects, suggesting that these motivations are less persistent.

There are a few cross AR effects that have a reasonable impact: the largest odds ratio of 1.254 is from motivation 81 on 95. Motivation 95 relates to rental charges and waivers, whereas the most likely product in motivation 81 is an e-deposit product with purchase probability of 0.499. It is very plausible that if motivation 81 is activated it becomes more likely that motivation 95 will become active in the next shopping trip. This does not hold the other way around, because the asymmetric cross AR effect from motivation 95 on 81 is much closer to unity (1.035). The next largest cross AR effect that we find is much smaller, 1.048, and relates to motivation 21 (installation of irrigation systems) and motivation 17 (Plumbing - PVC pipes: 1/2'' and 3/4''). Again, it seems reasonable that these two motivations are related. Furthermore, this relationship is more symmetric as the cross AR effect from motivation 17 on motivation 21 is 1.045.

Although there is some variation among the cross AR effects, most odds ratios are located around unity. Hence, in our application, we do not find many cases where one motivation starkly increases—or decreases—the probability of another motivation at the next shopping

trip. A potential explanation is that in our empirical application, relationships between motivations mainly exist at the customer level, and not over time within a customer. Such relationships are absorbed in the heterogeneity covariance matrix Σ_κ . In other empirical applications, however, path dependence in motivation activation could be more important.

5.5. Predictive Performance

To determine the predictive performance of the model, we use the holdout data set that contains the last shopping trip for every customer that has visited the store more than once. This data set is denoted by \mathbf{y}^{OOS} . We measure predictive performance of a model on this holdout data by evaluating $\log p(\mathbf{y}^{\text{OOS}}|\mathbf{y})$: the log predictive likelihood of \mathbf{y}^{OOS} conditional on the estimation data \mathbf{y} .

We contrast the predictive performance of our model against several competing methods. First, to better assess the added value of the VAR(1) effects, we consider our own model without these effects. Second, we consider a version of the latent Dirichlet allocation with explanatory variables (LDA-X) model (Jacobs et al. 2016) that is nested within our model, see Section 2.4, which aggregates over trips and therefore does not include any trip-specific information. It also ignores correlations between the motivations. Finally, to place the performance of these models into perspective, we consider two model-free benchmarks without customer heterogeneity: a marginal probability vector where the probabilities are based on the relative purchase frequencies in the estimation data and a naive flat probability vector where each product has a purchase probability of J^{-1} .

The predictive performance results are displayed in Table 8. Our model clearly outperforms the alternatives. The LDA-X model is outperformed by a margin of more than 1,000 log-likelihood points. A large driver of this performance increase are the time effects and motivation correlations that result in a more realistic model. Furthermore, the VAR(1) effects in our model provide a positive contribution to the model's predictive performance as well, which validates their inclusion in the model. In addition, the results clearly show that all models outperform the model-free benchmarks.

6. Managerial Implications

One of the key strengths of our model is that it identifies purchase motivations from purchase history data alone. These motivations provide a novel view on purchase behavior, exposing the salient purchase patterns and how these differ across customers and shopping trips. This is especially useful for retailers with large product assortments, in which such purchase patterns can be obfuscated because of the volume of purchases and variety of the product assortment. In such cases, considering customer behavior expressed through purchase motivations is simpler, more intuitive, and may lead to better insights. In this section, we discuss how the model results, and in particular the motivations, can serve as input to managerial decisions.

Managerial dashboards: All the insights we generated in the previous section are helpful in managerial decision making. The model results provide company experts detailed, quantified knowledge on the customer base and product assortment. To facilitate the discovery of relevant insights one could easily build a managerial model-based dashboard around the model results. The focal perspective of such a dashboard may be based on a product, a motivation, a time period, or even an individual customer. A dashboard for a specific product may contain a ranking of motivations, for example, displaying the five most likely motivations for that product.

A dashboard can also be constructed for a specific motivation. Naturally, the most likely products under that motivation can be displayed, which allows for the creation of intuitive labels for the motivations. In addition, the motivations that correlate most strongly with the focal motivation can be listed. Yet another insight in a specific motivation is given by seasonality and the effects of the explanatory variables such as customer age and gender. Such effects provide a detailed picture on when—and for whom—a motivation is most likely active. Conversely, it is possible to list the most relevant motivations for a given customer segment at a certain point in time.

Explainable product recommendations: The model structure can serve as the basis for explainable product recommendations at a retailer. At the highest level, an explanation for the recommended products can be provided through a link with the activated motivations that drive the product recommendation. At a more

Table 8. Log Predictive Likelihood of the Holdout Data for Different Methods

Model	\mathbf{w}_i	\mathbf{x}_{ib}	Correlations	VAR(1)	$\log p(\mathbf{y}^{\text{OOS}} \mathbf{y})$
Complete model	x	x	X	X	-40,517.69
Model without VAR(1) effects	X	X	X	_	-40,541.65
LDA-X	х	_	_	_	-41,545.51
Marginal probability vector	_	_	_	_	-43,814.22
Flat probability vector	_	_	_	_	-46,581.54

detailed level, the model output can be used to explain the predicted relevance of the motivations for the customer's shopping trip. Specifically, a selection of the most important explanatory variables such as a customer's innate preferences, demographics, the context of the shopping trip, or the contents of the previous shopping trip, can be used to explain why these motivations are predicted to be active. This provides a detailed, yet understandable explanation why certain motivations are active for a customer and hence, why certain products are expected to be relevant for that customer. Common recommendation systems, such as matrix factorization techniques, cannot provide such insights.

Targeted advertising: The inferred motivations also provide opportunities for targeted advertising and the specific timing of such actions. Targeted advertising can even be applied within the store. As an example of such a real-time action, consider a *smart shopping cart*. This shopping cart may contain a device that registers when a customer places a product in her shopping cart. The relevant motivations corresponding to this product can be identified and this information can be directly communicated to the customer, for example, on the shopping cart or on their mobile phone.

In the context of a hardware store, such information can be an instructional video that explains how to complete a do-it-yourself project corresponding to the motivation. More generally, a list of relevant products, based on the motivation, or a promotion tailored to the motivation can be shown. Opportunities for personalized communication continue after a shopping trip has ended. For example, consider timely follow-up (e)mails that promote motivations that have become more relevant after a shopping trip. Such motivations can be determined using the inferred motivation-correlations and the VAR(1)-effects.

Knowing which motivations are (ir)relevant for a customer can also improve communication with the customer. If a customer is likely to engage in do-ityourself home improvement projects but has shown little interest in gardening motivations, marketing campaigns directed at this customer can be adjusted accordingly. Reaching out to customers at the level of their motivations is preferred over communication at the product level for at least two reasons. First, given the large size of the product assortment, it is quite unlikely to accurately predict the specific product the customer wants to buy. Predicting the correct motivation is much more realistic and hence this might be more effective in engaging the customer. Second, communicating at a higher level in terms of the purchase motivations—instead of at the detailed product level—is more appreciated by customers, especially when the communication is not immediately linked to a purchase decision (da Costa Hernandez et al. 2015).

Improving store layout: Insights about the relevant motivations can be used to improve store layouts,

both for online and offline stores. First consider a brick-and-mortar store: small products that are relevant across multiple motivations can be positioned strategically at multiple places within the store to improve the shopping experience. As an example, work gloves are relevant for gardening activities, but also for renovation jobs. By placing the work gloves in both locations in the store, they become easier to locate for customers. Additionally, the correlations between motivations could be used to position product categories in a store relative to each other. For example, if certain PVC pipes are most often used in a bathroom renovation, it may make sense to position those PVC pipes relatively close to products such as toilets, bathtubs, and showers.

Similarly, inferred motivations can be used in an online store. For example, for each motivation a landing page can be created, containing both products and other motivations which are related to the focal motivation. As an example, consider a landing page specific to a barbecue motivation. Not only would the relevant products be displayed, such as grills and utensils, but relevant motivations could be linked as well, such as motivations related to insect repellents or an outdoor pool. Our model is able to identify the most related motivations. In a similar vein, a product page can refer to motivations under which the product is likely to be purchased. As one of these motivations is likely to be relevant, linking to that motivation can create promising cross-selling opportunities.

Another approach is to link (sponsored) search queries to motivations. For each search query that does not exactly match a specific product, one can identify the best matching motivation. A landing page related to a motivation will likely outperform a landing page that only lists a single product. In this way, one would directly connect the customer to the full set of products the customer is interested in, which again provides clear opportunities for cross-selling.

There are other benefits to identifying purchase motivations that are not directly connected to marketing actions. As an example, consider inventory management. A promotion for a certain product may create spillover effects to other products. Using motivations, these spillover effects can be anticipated. This example, and those presented above, all seem to benefit from a succinct representation of purchase behavior, expressed using a small set of motivations. We consider the actual application of motivation-assisted marketing decision making a very exciting and fruitful avenue for further research.

7. Conclusions and Further Research

In this paper, we have introduced a novel model that efficiently analyzes large-scale purchase history data,

consisting of product purchase decisions made by many customers—in an even larger number of shopping trips—out of a product assortment consisting of thousands of products. Using the model, we extract insights relevant for marketing decision makers and help determine the salient purchase patterns to improve understanding of purchase behavior in the customer base. The fundamental idea is to represent the high-dimensional purchase data in a lower-dimensional space, spanned by latent purchase motivations. The motivations are incorporated in the model as probability distributions over the product assortment, which are identified using only observational purchase history data: data that are ubiquitous in modern retail applications. The model results can be used to formalize and quantify how probabilities for motivation activation and product purchases are linked to and affected by explanatory variables, such as seasonality or customer demographics.

The model is designed such that it scales well to realistic retail settings, ensuring that it can be used to generate valuable insights in practice. We have achieved this in several ways. First, the model is built on the class of topic models, which is known to scale well to large applications. Second, to estimate the model parameters we rely on an estimation technique from the machine learning literature called variational inference. This technique has proven successful for estimating large and complex models in a reasonable time frame. Third, we extend results from the variational inference literature, by deriving a novel algorithm that can be used to efficiently estimate a large motivation-covariance matrix for applications with many motivations.

In the current model, we only rely on off-the-shelf purchase history data to identify the purchase motivations structure. Although this modeling decision makes the model easy to adopt in practice, it also has some limitations. Purchases made by customers are partially affected by factors under the control of a retailer, for example, product prices, promotion strategies, and store layout. Controlling for these factors in the inference of the motivations is a promising avenue for further research.

Another direction for further research is product recommendations based on the inferred motivations. In this paper, we have shown that our model is able to accurately predict purchases in the next shopping trip. A next step would be to incorporate these predictions in a product recommendation system. The benefit of such a recommendation system is that it leads to product recommendations that can be explained in terms of motivations and explanatory variables. However, a product that is likely to be purchased by a customer is not necessarily an effective recommendation (Bodapati 2008). The effectiveness of recommendations based on purchase motivations is an open empirical question.

Developing and implementing marketing actions based on the inferred motivations provides another direction for further research. In this paper, we have shown that our model is able to capture meaningful motivations at the customer level and across the shopping trips of a single customer. The inferred motivation structure also results in accurate predictions of a customer's purchases in the next shopping trip. Future research could implement and study the effectiveness of marketing actions that build on the insights generated by our model, such as landing pages tailored to the most likely motivation, or a recommendation system that is based on accurate, explainable predictions. In sum, we see our model as an important tool for the analysis of purchase behavior in high-dimensional retail settings and as a stepping stone for motivation-based marketing actions at retailers with large assortments.

Appendix

Notation

We use the following notation to facilitate exposition in the appendices of this paper:

- [x]: The Iverson Bracket, equal to 1 if x is True, else 0
- $\mathcal{I}[z]$ with $z \in \{1, ..., M\}$: An M-dimensional vector of zeros in which the zth element is set to 1
 - $d(\mathbf{v})$: Creates a diagonal matrix out of the vector \mathbf{v}
- $\tilde{\mathbb{E}}\{\vartheta\}$: Expectation of parameter ϑ under its variational distribution $q(\vartheta)$, that is, $\tilde{\mathbb{E}}\{\vartheta\} \equiv \mathbb{E}_{q(\vartheta)}\{\vartheta\}$
- I: Identity matrix; 1: vector of ones; 0: vector of zeros. The dimension is indicated by a subscript

Appendix A. Additional Model Details

This appendix describes additional model details: a specification of the motivation relevance for the first shopping trip and the prior distributions for all population-level parameters in the model.

The motivation relevance for shopping trip b made by customer i, α_{ib} , is modeled as a function of the previous shopping trip: α_{ib-1} (cf. Equation (4)). This lagged value is not available if b refers to the first (observed) shopping trip of a customer. For these shopping trips we specify an adjusted model for the expected motivation relevance:

$$\mu_{i1m} = \delta_m + \delta_\kappa \kappa_{im} + \delta_\beta \mathbf{x}_{i1}^\mathsf{T} \boldsymbol{\beta}_m + \delta_\gamma \mathbf{w}_i^\mathsf{T} \boldsymbol{\gamma}_m, \tag{A.1}$$

where δ_m is a motivation-specific intercept. In addition, δ_κ , δ_β and δ_γ are scalar factors that allow for shifts in effect sizes that are specific to the first shopping trip of a customer. Because these three parameters reflect proportional shifts, their priors are centered around unity instead of zero.

For the specification of the prior, we transform variance parameters to their inverse, that is, precision parameters. More specifically, the variance for ϵ_{ibm} , $\sigma^2_{\alpha_m}$ is transformed to a precision $\tau_{\alpha_m} \equiv \sigma^{-2}_{\alpha_m}$, with $\tau_{\alpha} = [\tau_{\alpha_1}, \ldots, \tau_{\alpha_M}]$. The covariance matrix for κ_i , Σ_{κ} , is transformed to a precision matrix $\Lambda_{\kappa} \equiv \Sigma_{\kappa}^{-1}$. For each population parameter the prior is chosen such that it is conjugate to the parameter's full-conditional distribution. The parameters of the prior distributions are

set such that they represent relatively uninformative distributions. Large parameters inside a softmax function tend to result in implausible outcomes (see table 1 in Pachali et al. 2020 for a related conclusion), so a prior variance of 1 is already substantial. The priors for the population-level parameters are

```
For m = 1, ..., M:

\phi_m \sim \text{Dirichlet}_J(\alpha = \mathbf{1}_J J^{-1}),
\rho_m \sim \text{MVN}_M(\mu = \mathbf{0}_M, \Sigma = \mathbf{I}_M),
\beta_m \sim \text{MVN}_{K_X}(\mu = \mathbf{0}_{K_X}, \Sigma = \mathbf{I}_{K_X}),
\gamma_m \sim \text{MVN}_{K_W}(\mu = \mathbf{0}_{K_W}, \Sigma = \mathbf{I}_{K_W}),
\delta_m \sim \text{Normal}(\mu = 0, \sigma^2 = 1),
\tau_{\alpha_m} \sim \text{Gamma}(\alpha = 1, \beta = 1),
\delta_K, \delta_\beta, \delta_\gamma \sim \text{Normal}(\mu = 1, \sigma^2 = 1),
\mu_K \sim \text{MVN}_M(\mu = \mathbf{0}_M, \Sigma = \mathbf{I}_M),
\Lambda_K \sim \text{Wishart}_M(n = 2M, \mathbf{V} = \mathbf{I}_M(2M)^{-1}).
```

Appendix B. Estimation Details Using VI

This appendix contains the details for our estimation routine that uses VI to estimate the unknown model components. We start with pseudocode for the algorithm, after which we provide the update steps for each parameter's variational distribution.

The objective of VI is to minimize the KL divergence from $q(\Omega)$ to $p(\Omega|y)$ with respect to the parameters of the variational distribution. This is equivalent to maximizing the corresponding ELBO (Blei et al. 2017):

ELBO
$$\equiv \log p(\mathbf{y}) - \text{KL}\{q(\mathbf{\Omega}) || p(\mathbf{\Omega}|\mathbf{y})\}\$$

= $\tilde{\text{E}}\{\log p(\mathbf{y}, \mathbf{\Omega})\} + \text{ENTROPY}\{q(\mathbf{\Omega})\}.$ (B.1)

The pseudocode to maximize the ELBO of our model is given in Algorithm B.1. After each update step in the algorithm, the ELBO is guaranteed to not decrease. Per iteration and for each customer i, we take L=25 subiterations to jointly optimize the variational distributions specific to customer i. The optimization is completed once the ELBO has converged.

Algorithm B.1. Pseudocode for VI Coordinate Ascent Optimization Algorithm

```
1: Initialize q(\Omega)
  2: while ELBO has not converged do
  3:
            for i = 1, ..., I do
                 for \ell = 1, \ldots, L do
  4:
  5:
                      for b = 1, ..., N_{ib} do
  6:
                           Update q(\mathbf{z}_{ib}), q(\boldsymbol{\alpha}_{ib})
  7:
                      end for
  8:
                      Update q(\kappa_i)
  9:
                 end for
10:
11:
            Update q(\boldsymbol{\phi}), q(\boldsymbol{\beta}), q(\boldsymbol{\gamma}), q(\boldsymbol{\rho}), q(\boldsymbol{\delta}), q(\delta_{\kappa}), q(\delta_{\beta}), q(\delta_{\gamma}), q(\tau_{\alpha}),
                  q(\boldsymbol{\mu}_{\kappa}), q(\boldsymbol{\Lambda}_{\kappa})
12: end while
```

B.1. Variational Updates

The specification of $\epsilon_{ibm} \equiv \alpha_{ibm} - \mu_{ibm}$ and $\epsilon_{ib} \equiv [\epsilon_{ib1}, \dots, \epsilon_{ibM}]$ plays a central role in the variational updates for α_{ib} and all the parameters in the Markov blanket¹⁰ for α_{ib} . The relevant variational expectations of ϵ_{ibm} are defined as

$$\tilde{\mathbf{E}}\{\epsilon_{ibm}\} \equiv \tilde{\mathbf{E}}\{\alpha_{ibm}\} - \tilde{\mathbf{E}}\{\mu_{ibm}\},
\tilde{\mathbf{E}}\{\epsilon_{ibm}^2\} \equiv \tilde{\mathbf{E}}\{\alpha_{ibm}^2\} + \tilde{\mathbf{E}}\{\mu_{ibm}^2\} - 2\tilde{\mathbf{E}}\{\alpha_{ibm}\}\tilde{\mathbf{E}}\{\mu_{ibm}\}.$$
(B.2)

Based on the specification of μ_{ibm} in Equation (4), we obtain

$$\tilde{\mathbf{E}}\{\boldsymbol{\mu}_{ib}\} = \tilde{\mathbf{E}}\{\boldsymbol{\kappa}_i\} + \tilde{\mathbf{E}}\{\mathbf{R}\}\tilde{\mathbf{E}}\{\boldsymbol{\alpha}_{ib-1}\} + \tilde{\mathbf{E}}\{\mathbf{B}\}\boldsymbol{x}_{ib} + \tilde{\mathbf{E}}\{\mathbf{G}\}\boldsymbol{w}_{i}, \quad (B.3)$$

with $\mu_{ib} \equiv [\mu_{ib1}, \dots, \mu_{ibM}]$ and where the ρ_m , β_m , and γ_m vectors have been collected in the matrices \mathbf{R} , \mathbf{B} , and \mathbf{G} that are, respectively, of dimensions $M \times M$, $M \times K_X$, and $M \times K_W$. In other words, the mth row of each matrix corresponds to parameters ρ_m , β_m , and γ_m , respectively.

We start by introducing notation to facilitate a concise exposition of our results. We often need to compute variational moments of α_{ib} cleaned from the explained effect of all but one of the factors in μ_{ib} . To illustrate this with an example, we can clean α_{ib} of the effect of all factors except κ_i as follows:

$$\alpha_{ib} - \mathbf{R}\alpha_{ib-1} - \mathbf{B}\mathbf{x}_{ib} - \mathbf{G}\mathbf{w}_i = \alpha_{ib} - (\mu_{ib} - \kappa_i)$$

$$= (\alpha_{ib} - \mu_{ib}) + \kappa_i$$

$$\equiv \langle \epsilon_{ib} + \kappa_i \rangle.$$

Writing the cleaned effect as $\epsilon_{ib} + \kappa_i$ simplifies notation and is an efficient way to calculate the cleaned effect. To emphasize that result $\epsilon_{ib} + \kappa_i$ is in fact not dependent on κ_i , we place it between angle brackets. Variational moments of $\langle \epsilon_{ib} + \kappa_i \rangle$ therefore do not depend on $q(\kappa_i)$.

We introduce notation to stack the \mathbf{x}_{ib} , \mathbf{w}_i , $\boldsymbol{\epsilon}_{ib}$, and $\boldsymbol{\alpha}_{ib}$ vectors into matrices. $\mathbf{X}_{(1)}$ stacks the \mathbf{x}_{ib} vectors that correspond with a first shopping trip in an $I \times K_X$ matrix. The same notation applies for \mathbf{w}_i ($\mathbf{W}_{(1)}$) and $\boldsymbol{\epsilon}_{ib}$ ($\mathbf{E}_{(1)}$). Similarly, $\mathbf{X}_{(2+)}$ stacks the remaining \mathbf{x}_{ib} vectors that do not correspond with a first shopping trip in an $((\sum_{i=1}^{I} B_i) - I) \times K_X$ matrix. Again, the same notation applies for $\boldsymbol{\epsilon}_{ib}$ ($\mathbf{E}_{(2+)}$) and \mathbf{w}_i ($\mathbf{W}_{(2+)}$), where $\mathbf{W}_{(2+)}$ contains $B_i - 1$ duplicated rows \mathbf{w}_i for each customer i. In addition, the mth columns of $\mathbf{E}_{(1)}$ and $\mathbf{E}_{(2+)}$ are denoted by $\mathbf{e}_{(1),m}$ and $\mathbf{e}_{(2+),m}$. Last, $\mathbf{A}_{(-1)}$ stacks all $\boldsymbol{\alpha}_{ib}$ vectors that do not correspond to a last shopping trip, in a $((\sum_{i=1}^{I} B_i) - I) \times M$ matrix.

Our model specification only consists of distributions from the exponential family and we apply mean-field VI with a partitioning $F(\Omega)$ that retains all elements of a multivariate parameter within a single subset, ω , for all multivariate parameters in the model. This allows us to use known results from the VI literature to directly write down a general expression for the optimal variational distribution $q^*(\omega)$ for each conditionally conjugate parameter in Ω , given all other variational distributions. In our model, all parameters except α_{ib} are conditionally conjugate.

B.1.1. Closed-Form Solutions for the Variational Updates.

We use the general form of the optimal variational distribution under the mean-field assumption (Bishop 2006), applied to distributions in the exponential family (Blei et al. 2017). Given that ω is a conditionally conjugate parameter in the model and that ω is distributed according to a distribution from the exponential family, it holds that the optimal variational distribution for ω is given by

$$q^{\star}(\omega) \propto h(\omega) \exp(t(\omega)^{\top} \tilde{\mathbf{E}}_{\mathrm{MB}_{\omega}} \{ \eta(\mathrm{MB}_{\omega}) \}).$$
 (B.4)

Here h and t are functions that match the functional form corresponding to the base measure and the sufficient statistic of the prior distribution for ω in the model, and MB_ω refers to the Markov blanket for ω . $\eta(\mathrm{MB}_\omega)$ is the natural parameter corresponding to the full-conditional distribution $p(\omega|\mathrm{MB}_\omega)$. Its variational expectation, $\tilde{\mathrm{E}}_{\mathrm{MB}_\omega}\{\eta(\mathrm{MB}_\omega)\}$, is the natural parameter corresponding to the optimal variational distribution $q^*(\omega)$. Evaluating this expectation only requires the variational distributions of the parameters in the Markov blanket for ω . We apply (B.4) to directly write down the updates for all conditionally conjugate parameters in the model. In the updates corresponding to a population-level parameter, any literal values such as a 0,1, or the identity matrix \mathbf{I} , correspond to the fixed values of the prior parameters as specified in Appendix A.

Update $q(z_{ibn})$: M-dimensional Categorical with probability that $z_{ibn} = m$ given by

$$\tilde{p}_{ibnm} = \frac{\exp\left(\tilde{E}\{\alpha_{ibm}\} + \tilde{E}\{\log \phi_{m,y_{ibn}}\}\right)}{\sum_{\ell=1}^{M} \exp\left(\tilde{E}\{\alpha_{ib\ell}\} + \tilde{E}\{\log \phi_{\ell,y_{ibn}}\}\right)}.$$
 (B.5)

Update $q(\phi_m)$: *J*-dimensional Dirichlet with parameter $\tilde{\mathbf{a}}_m$ for which the *j*th element is specified as

$$\tilde{a}_{mj} = J^{-1} + \sum_{i} \sum_{h=1}^{B_i} \sum_{n=1}^{N_{th}} \tilde{E}\{[z_{ibn} = m]\}[y_{ibn} = j].$$
 (B.6)

Update $q(\tau_{\alpha_m})$: Gamma with parameters

$$\tilde{a}_{\tau_{\alpha_m}} = 1 + \frac{1}{2} \sum_{i} B_i, \quad \tilde{b}_{\tau_{\alpha_m}} = 1 + \frac{1}{2} \sum_{i} \sum_{b=1}^{B_i} \tilde{E}\{\epsilon_{ibm}^2\}.$$
 (B.7)

Update $q(\Lambda_{\kappa})$: *M*-dimensional Wishart with parameters

$$\tilde{\mathbf{N}}_{\Lambda_{\kappa}} = 2M + I,$$

$$\tilde{\mathbf{V}}_{\Lambda_{\kappa}} = \left(\mathbf{I}_{M}(2M) + \sum_{i} \tilde{\mathbf{E}} \left\{ \boldsymbol{\mu}_{\kappa} \boldsymbol{\mu}_{\kappa}^{\top} + \boldsymbol{\kappa}_{i} \boldsymbol{\kappa}_{i}^{\top} - \boldsymbol{\mu}_{\kappa} \boldsymbol{\kappa}_{i}^{\top} - \boldsymbol{\kappa}_{i} \boldsymbol{\mu}_{\kappa}^{\top} \right\} \right)^{-1}.$$
(B.8)

Update $q(\kappa_i)$: *M*-dimensional multivariate Normal with parameters

$$\tilde{\Sigma}_{i} = \tilde{\mathbb{E}} \left\{ \Lambda_{\kappa} + d(\tau_{\alpha}) \left(\delta_{\kappa}^{2} + B_{i} - 1 \right) \right\}^{-1},
\tilde{\mu}_{i} = \tilde{\Sigma}_{i} \tilde{\mathbb{E}} \left\{ \Lambda_{\kappa} \mu_{\kappa} + d(\tau_{\alpha}) \left(\delta_{\kappa} \langle \epsilon_{i1} + \kappa_{i} \delta_{\kappa} \rangle + \sum_{b=2}^{B_{i}} \langle \epsilon_{ib} + \kappa_{i} \rangle \right) \right\}.$$
(B.9)

Update $q(\beta_m)$: K_X -dimensional multivariate Normal with parameters

$$\tilde{\boldsymbol{\Sigma}}_{\beta_{m}} = \tilde{\mathbf{E}} \Big\{ \mathbf{I}_{K_{X}} + \Big(\mathbf{X}_{(1)}^{\top} \mathbf{X}_{(1)} \delta_{\beta}^{2} + \mathbf{X}_{(2+)}^{\top} \mathbf{X}_{(2+)} \Big) \boldsymbol{\tau}_{\alpha_{m}} \Big\}^{-1},
\tilde{\boldsymbol{\mu}}_{\beta_{m}} = \tilde{\boldsymbol{\Sigma}}_{\beta_{m}} \tilde{\mathbf{E}} \Big\{ \mathbf{0}_{K_{X}} + \boldsymbol{\tau}_{\alpha_{m}} \Big(\delta_{\beta} \mathbf{X}_{(1)}^{\top} \langle \mathbf{e}_{(1),m} + \mathbf{X}_{(1)} \boldsymbol{\beta}_{m} \delta_{\beta} \rangle
+ \mathbf{X}_{(2+)}^{\top} \langle \mathbf{e}_{(2+),m} + \mathbf{X}_{(2+)} \boldsymbol{\beta}_{m} \rangle \Big) \Big\}.$$
(B.10)

Update $q(\gamma_m)$: K_W -dimensional multivariate Normal with parameters

$$\begin{split} \tilde{\boldsymbol{\Sigma}}_{\gamma_{m}} &= \tilde{\mathbf{E}} \Big\{ \mathbf{I}_{K_{W}} + \Big(\mathbf{W}_{(1)}^{\top} \mathbf{W}_{(1)} \delta_{\gamma}^{2} + \mathbf{W}_{(2+)}^{\top} \mathbf{W}_{(2+)} \Big) \boldsymbol{\tau}_{\alpha_{m}} \Big\}^{-1}, \\ \tilde{\boldsymbol{\mu}}_{\gamma_{m}} &= \tilde{\boldsymbol{\Sigma}}_{\gamma_{m}} \tilde{\mathbf{E}} \Big\{ \mathbf{0}_{K_{W}} + \boldsymbol{\tau}_{\alpha_{m}} \Big(\delta_{\gamma} \mathbf{W}_{(1)}^{\top} \langle \mathbf{e}_{(1),m} + \mathbf{W}_{(1)} \boldsymbol{\gamma}_{m} \delta_{\gamma} \rangle \\ &+ \mathbf{W}_{(2+)}^{\top} \langle \mathbf{e}_{(2+),m} + \mathbf{W}_{(2+)} \boldsymbol{\gamma}_{m} \rangle \Big) \Big\}. \end{split}$$
(B.11)

Update $q(\rho_m)$: M-dimensional multivariate Normal with parameters

$$\tilde{\boldsymbol{\Sigma}}_{\rho_{m}} = \tilde{\mathbf{E}} \Big\{ \mathbf{I}_{M} + \mathbf{A}_{(-1)}^{\mathsf{T}} \mathbf{A}_{(-1)} \boldsymbol{\tau}_{\alpha_{m}} \Big\}^{-1},
\tilde{\boldsymbol{\mu}}_{\rho_{m}} = \tilde{\boldsymbol{\Sigma}}_{\rho_{m}} \tilde{\mathbf{E}} \Big\{ \mathbf{0}_{M} + \boldsymbol{\tau}_{\alpha_{m}} \mathbf{A}_{(-1)}^{\mathsf{T}} \langle \mathbf{e}_{(2+),m} + \mathbf{A}_{(-1)} \boldsymbol{\rho}_{m} \rangle \Big\}.$$
(B.12)

Update $q(\mu_{\kappa})$: *M*-dimensional multivariate Normal with parameters

$$\tilde{\Sigma}_{\mu_{k}} = \tilde{\mathbb{E}} \{ \mathbf{I}_{M} + \mathbf{\Lambda}_{\kappa} I \}^{-1},
\tilde{\mu}_{\mu_{\kappa}} = \tilde{\Sigma}_{\mu_{k}} \tilde{\mathbb{E}} \left\{ \mathbf{0}_{M} + \mathbf{\Lambda}_{\kappa} \sum_{i} \kappa_{i} \right\}.$$
(B.13)

Update $q(\delta_m)$: Normal with parameters

$$\tilde{\sigma}_{\delta_{m}}^{2} = \tilde{E}\left\{1 + \tau_{\alpha_{m}}I\right\}^{-1},
\tilde{\mu}_{\delta_{m}} = \tilde{\sigma}_{\delta_{m}}^{2}\tilde{E}\left\{0 + \tau_{\alpha_{m}}\sum_{i}\langle\epsilon_{i1m} + \delta_{m}\rangle\right\}.$$
(B.14)

Update $q(\delta_{\kappa})$: Normal with parameters

$$\begin{split} \tilde{\sigma}_{\delta_{\kappa}}^{2} &= \tilde{\mathbf{E}} \left\{ 1 + \sum_{m} \tau_{\alpha_{m}} \sum_{i} \kappa_{im}^{2} \right\}^{-1}, \\ \tilde{\mu}_{\delta_{\kappa}} &= \tilde{\sigma}_{\delta_{\kappa}}^{2} \tilde{\mathbf{E}} \left\{ 1 + \sum_{m} \tau_{\alpha_{m}} \sum_{i} \kappa_{im} \langle \epsilon_{i1m} + \kappa_{im} \delta_{\kappa} \rangle \right\}. \end{split} \tag{B.15}$$

Update $q(\delta_{\beta})$: Normal with parameters

$$\tilde{\sigma}_{\delta_{\beta}}^{2} = \tilde{E} \left\{ 1 + \operatorname{tr} \left(\mathbf{X}_{(1)}^{\top} \mathbf{X}_{(1)} \sum_{m} \tau_{\alpha_{m}} \boldsymbol{\beta}_{m} \boldsymbol{\beta}_{m}^{\top} \right) \right\}^{-1},$$

$$\tilde{\mu}_{\delta_{\beta}} = \tilde{\sigma}_{\delta_{\beta}}^{2} \tilde{E} \left\{ 1 + \sum_{m} \tau_{\alpha_{m}} \boldsymbol{\beta}_{m}^{\top} \mathbf{X}_{(1)}^{\top} \langle \mathbf{e}_{(1),m} + \mathbf{X}_{(1)} \boldsymbol{\beta}_{m} \delta_{\beta} \rangle \right\}. \tag{B.16}$$

Update $q(\delta_{\gamma})$: Normal with parameters

$$\tilde{\sigma}_{\delta_{\gamma}}^{2} = \tilde{\mathbf{E}} \left\{ 1 + \operatorname{tr} \left(\mathbf{W}_{(1)}^{\top} \mathbf{W}_{(1)} \sum_{m} \tau_{\alpha_{m}} \boldsymbol{\gamma}_{m} \boldsymbol{\gamma}_{m}^{\top} \right) \right\}^{-1},$$

$$\tilde{\mu}_{\delta_{\gamma}} = \tilde{\sigma}_{\delta_{\gamma}}^{2} \tilde{\mathbf{E}} \left\{ 1 + \sum_{m} \tau_{\alpha_{m}} \boldsymbol{\gamma}_{m}^{\top} \mathbf{W}_{(1)}^{\top} \langle \mathbf{e}_{(1),m} + \mathbf{W}_{(1)} \boldsymbol{\gamma}_{m} \delta_{\gamma} \rangle \right\}. \quad (B.17)$$

B.1.2. Variational Update for $q(\alpha_{ib})$. Because α_{ib} is not a conditionally conjugate parameter in the model, an analytical solution for its optimal variational distribution does not exist. Instead, we place $q(\alpha_{ib})$ in the prior family for α_{ib} , i.e. a set of independent Normal distributions, with variational parameters $\tilde{\mu}_{ib}$ and $\tilde{\sigma}_{ib}^2$. In the optimization algorithm,

we rely on gradient information to update these $\tilde{\mu}_{ih}$ and $\tilde{\sigma}_{ih}^2$ parameters. To derive these gradients, we first define the part of the ELBO that depends on the variational parameters $\tilde{\mu}_{ib}$ and $\tilde{\sigma}_{ib}^2$ of $q(\alpha_{ib})$ as

$$\begin{split} \text{ELBO}_{ib} &= -\frac{1}{2} \big(\tilde{\sigma}_{ib}^2 + \tilde{\mu}_{ib}^2 \big)^\top \tilde{\mathbf{E}} \{ \boldsymbol{\tau}_{\alpha} \} \\ &+ \tilde{\mu}_{ib}^\top \bigg(\tilde{\mathbf{E}} \{ \boldsymbol{\tau}_{\alpha} \} \cdot \tilde{\mathbf{E}} \{ \boldsymbol{\mu}_{ib} \} + \sum_{n=1}^{N_{ib}} \tilde{\mathbf{E}} \{ \mathcal{I}[\boldsymbol{z}_{ibn}] \} \bigg) \\ &+ \frac{1}{2} \sum_{m} \log \tilde{\sigma}_{ibm}^2 \\ &- N_{ib} \log \sum_{m} \exp \bigg(\tilde{\mu}_{ibm} + \frac{1}{2} \tilde{\sigma}_{ibm}^2 \bigg) - \frac{1}{2} [\boldsymbol{b} \neq \boldsymbol{B}_i] \\ &\times \operatorname{tr} \bigg((\boldsymbol{d}(\tilde{\sigma}_{ib}^2) + \tilde{\mu}_{ib} \tilde{\mu}_{ib}^\top) \sum_{m} \tilde{\mathbf{E}} \{ \boldsymbol{\tau}_{\alpha_m} \} \; \tilde{\mathbf{E}} \{ \boldsymbol{\rho}_m \boldsymbol{\rho}_m^\top \} \bigg) \\ &+ [\boldsymbol{b} \neq \boldsymbol{B}_i] \big(\tilde{\mathbf{E}} \{ \boldsymbol{\tau}_{\alpha} \} \cdot \tilde{\mathbf{E}} \{ \langle \boldsymbol{\epsilon}_{ib+1} + \mathbf{R} \boldsymbol{\alpha}_{ib} \rangle \} \big)^\top \; \tilde{\mathbf{E}} \{ \mathbf{R} \} \tilde{\boldsymbol{\mu}}_{ib}, \end{split} \tag{B.18}$$

where we have applied Jensen's Inequality to lower bound $-\mathbb{E}\{\log \sum_{m} \exp \alpha_{ibm}\}$, that is, the variational expectation of the log of the denominator of the softmax function, with $-\log \sum_m \tilde{E}\{\exp \alpha_{ibm}\}$ (Braun and McAuliffe 2010). The gradient of (B.18) with respect to $\tilde{\mu}_{ih}$ is given by

$$\nabla_{\tilde{\boldsymbol{\mu}}_{ib}} \text{ELBO}_{ib} = \tilde{\mathbb{E}} \{ \boldsymbol{\tau}_{\alpha} \} \cdot (\tilde{\mathbb{E}} \{ \boldsymbol{\mu}_{ib} \} - \tilde{\boldsymbol{\mu}}_{ib}) + \sum_{n=1}^{N_{ib}} \tilde{\mathbb{E}} \{ \mathcal{I}[\boldsymbol{z}_{ibn}] \}$$

$$- N_{ib} \frac{\exp(\tilde{\boldsymbol{\mu}}_{ib} + \frac{1}{2} \tilde{\boldsymbol{\sigma}}_{ib}^{2})}{\sum_{m} \exp(\tilde{\boldsymbol{\mu}}_{ibm} + \frac{1}{2} \tilde{\boldsymbol{\sigma}}_{ibm}^{2})}$$

$$- [\boldsymbol{b} \neq \boldsymbol{B}_{i}] \left(\sum_{m} \tilde{\mathbb{E}} \{ \boldsymbol{\tau}_{\alpha_{m}} \} \tilde{\mathbb{E}} \{ \boldsymbol{\rho}_{m} \boldsymbol{\rho}_{m}^{\top} \} \right) \tilde{\boldsymbol{\mu}}_{ib}$$

$$+ [\boldsymbol{b} \neq \boldsymbol{B}_{i}] \tilde{\mathbb{E}} \{ \mathbf{R} \}^{\top} (\tilde{\mathbb{E}} \{ \boldsymbol{\tau}_{\alpha} \} \cdot \tilde{\mathbb{E}} \{ \langle \boldsymbol{\epsilon}_{ib+1} + \mathbf{R} \boldsymbol{\alpha}_{ib} \rangle \}). \tag{B.19}$$

The gradient of (B.18) with respect to $\tilde{\sigma}_{ib}^2$ is given by

$$\begin{split} \nabla_{\tilde{\sigma}_{ib}^{2}} \text{ELBO}_{ib} &= -\frac{1}{2} \bigg(\tilde{\mathbb{E}} \{ \tau_{\alpha} \} - \tilde{\sigma}^{2} + N_{ib} \frac{\exp(\tilde{\mu}_{ib} + \frac{1}{2} \tilde{\sigma}_{ib}^{2})}{\sum_{m} \exp(\tilde{\mu}_{ibm} + \frac{1}{2} \tilde{\sigma}_{ibm}^{2})} \\ &+ [b \neq B_{i}] \mathbf{1}_{M} \sum_{m} \tilde{\mathbb{E}} \{ \tau_{\alpha_{m}} \} \tilde{\mathbb{E}} \{ \rho_{mm}^{2} \} \bigg). \end{split} \tag{B.20}$$

The pseudocode for the update for $q(\boldsymbol{\alpha}_{ib}) = \text{Normal}_{M}$ $(\mu = \tilde{\mu}_{ih}, \sigma^2 = \tilde{\sigma}_{ih}^2)$, is given in Algorithm B.2, where $q(MB_{\alpha_{ih}})$ refers to the variational distributions for the parameters in the Markov blanket of α_{ib} . The algorithm uses adaptive step sizes $ss_{ib}^{\tilde{\mu}}$ and $ss_{ib}^{\log \tilde{\sigma}}$. If a step in the direction of the gradient results in an increase (decrease) of the ELBO, the step size is multiplied (divided) by ss_{factor} . We restrict the adaptive step

sizes between ss_{min} and ss_{max} . In our implementation we take $ss_{\text{factor}} = 1.125$, $ss_{\text{min}} = 10^{-6}$, $ss_{\text{max}} = 1$.

Algorithm B.2. Pseudocode for Variational Update for $q(\alpha_{ib})$

1: **Input**:
$$\tilde{\mu}_{ib}$$
, $\tilde{\sigma}_{ib}^2$, $ss_{ib}^{\tilde{\mu}}$, $ss_{ib}^{\log \tilde{\sigma}}$, ss_{factor} , ss_{min} , ss_{max} , $q(\text{MB}_{\alpha_{ib}})$
2: Compute current ELBO contribution:
ELBO_{ib} = ELBO ($\tilde{\mu}_{ib}$, $\tilde{\sigma}_{ib}^2$ | $q(\text{MB}_{\alpha_{ib}})$)

3: Create candidate for
$$\tilde{\mu}_{ib}$$
:
$$\tilde{\mu}_{ib}^{\dagger} = \tilde{\mu}_{ib} + s s_{ib}^{\tilde{\mu}} \nabla_{\tilde{\mu}_{ib}} \text{ ELBO } (\tilde{\mu}_{ib}, \tilde{\sigma}_{ib}^2 | q(\text{MB}_{\alpha_{ib}}))$$
4: Compute candidate ELBO contribution:

$$ELBO_{ib}^{\dagger} = ELBO (\tilde{\boldsymbol{\mu}}_{ib}^{\dagger}, \tilde{\boldsymbol{\sigma}}_{ib}^{2} | q(MB_{\boldsymbol{\alpha}_{ib}})$$

4: Compute candidate ELBO contribution:

$$ELBO_{ib}^{\dagger} = ELBO \left(\tilde{\mu}_{ib}^{\dagger}, \tilde{\sigma}_{ib}^{2} | q(MB_{\alpha_{ib}}) \right)$$
5: **if** $ELBO_{ib}^{\dagger} > ELBO_{ib}$ **then**
6: Set $\tilde{\mu}_{ib} = \tilde{\mu}_{ib}^{\dagger}$ and $ELBO_{ib} = ELBO_{ib}^{\dagger}$
Increase ss_{ib}^{μ} : $ss_{ib}^{\bar{\mu}} = \min \left(ss_{factor}ss_{ib}^{\bar{\mu}}, ss_{max} \right)$

3: Decrease
$$ss_{ib}^{\tilde{\mu}}: ss_{ib}^{\tilde{\mu}} = \max(ss_{\text{factor}}^{-1} ss_{ib}^{\tilde{\mu}}, ss_{\text{min}})$$

10: Create candidate for $\log \tilde{\sigma}_{ib}$: $\log \tilde{\sigma}_{ib}^{\dagger} = \log \tilde{\sigma}_{ib} + s s_{ib}^{\log \tilde{\sigma}} 2 \tilde{\sigma}_{ib} \cdot \nabla_{\tilde{\sigma}_{ib}^2} \text{ELBO} \left(\tilde{\mu}_{ib'}, \tilde{\sigma}_{ib}^2 | q(\text{MB}_{\alpha_{ib}}) \right)$

11: Create candidate for $\tilde{\sigma}_{ib}^2$: $(\tilde{\sigma}_{ib}^2)^{\dagger} = \exp(2\log \tilde{\sigma}_{ib}^{\dagger})$

ELBO[†]_{ib} = ELBO
$$(\tilde{\mu}_{ib}, (\tilde{\sigma}_{ib}^2)^{\dagger} | q(MB_{\alpha_{ib}}))$$

13: **if**
$$ELBO_{ib}^{\dagger} > ELBO_{ib}$$
 then

13: if
$$\text{ELBO}_{ib}^{\dagger} > \text{ELBO}_{ib}$$
 then
14: Set $\tilde{G}_{ib}^{2} = (\tilde{G}_{ib}^{2})^{\dagger}$
Increase $ss_{ib}^{\log \tilde{\sigma}}: ss_{ib}^{\log \tilde{\sigma}} = \min(ss_{\text{factor}}ss_{ib}^{\log \tilde{\sigma}}, ss_{\text{max}})$

16: Decrease
$$ss_{ib}^{\log \tilde{\sigma}}$$
: $ss_{ib}^{\log \tilde{\sigma}} = \max(ss_{\text{factor}}^{-1} ss_{ib}^{\log \tilde{\sigma}}, ss_{\text{min}})$

18: **Output**:
$$\tilde{\boldsymbol{\mu}}_{ih}$$
, $\tilde{\sigma}_{ih}^2$, $ss_{ih}^{\tilde{\mu}}$, $ss_{ih}^{\log \tilde{\sigma}}$

B.2. Initialization of $q(\Omega)$

Algorithm B.1 requires initial values for the parameters of the variational distribution $q(\Omega)$. Because of the order in which the parameters are updated in Algorithm B.1, not all of these initial values will affect the outcome of the optimization. All (multivariate) Normal distributions are initialized with zero mean. For the population parameters with a Normal variational distribution for which the initial variance matters $(q(\rho_m), q(\delta_\kappa), q(\delta_\beta), q(\delta_\gamma))$, we initialize the variance to a small conservative value of M^{-2} to allow for a smooth optimization path. Additionally, these posterior distributions are expected to be sharply peaked, as a lot of information is available to estimate these population level parameters. In contrast, $q(\alpha_{ibm})$ is initialized with unit variance, as less information is available at the level of an individual shopping trip. $q(\tau_{\alpha_m})$ is initialized as Gamma($\alpha = 1, \beta = 1$), but we note that only the ratio α/β affects the outcome of the optimization. The variational distribution $q(\Lambda_{\kappa})$ is initialized as Wishart_M(n = 2M, V = $I(2M)^{-1}$). The initialization of $q(z_{ibn})$ has no effect. Finally, $q(\boldsymbol{\phi}_m)$ is initialized using pseudocounts from the output of a Collapsed Gibbs LDA algorithm applied to the data.

Appendix C. Proof for Efficient Covariance Matrix Inverse and (log) Determinant

Let \mathbf{M}_i be a $K \times K$ covariance matrix that is composed of two nonsingular $K \times K$ precision matrices \mathbf{P} and \mathbf{C} , where \mathbf{C} is multiplied by a non-negative scalar s_i :

$$\mathbf{M}_i \equiv (\mathbf{P} + \mathbf{C}s_i)^{-1}. \tag{C.1}$$

Both M_i and its determinant can be computed without inverting a $K \times K$ matrix that depends on s_i .

Proof M_i.

Step 1: Compute a Cholesky decomposition of $C: C = LL^T$ and rewrite M_i as

$$\mathbf{M}_{i} = (\mathbf{P} + \mathbf{L}\mathbf{L}^{\mathsf{T}}s_{i})^{-1}$$
$$= (\mathbf{L}(\mathbf{L}^{-1}\mathbf{P}(\mathbf{L}^{-1})^{\mathsf{T}} + \mathbf{I}s_{i})\mathbf{L}^{\mathsf{T}})^{-1}. \tag{C.2}$$

Step 2: Compute a singular value decomposition of $\mathbf{L}^{-1}\mathbf{P}(\mathbf{L}^{-1})^{\mathsf{T}}$ that is, $\mathbf{L}^{-1}\mathbf{P}(\mathbf{L}^{-1})^{\mathsf{T}} = \mathbf{U}d(\mathbf{v})\mathbf{U}^{\mathsf{T}}$, where $d(\mathbf{v})$ creates a diagonal matrix out of the vector \mathbf{v} . By design, $\mathbf{U}^{\mathsf{T}} = \mathbf{U}^{-1}$ and $\mathbf{U}\mathbf{U}^{\mathsf{T}} = \mathbf{U}\mathbf{U}^{-1} = \mathbf{I}$. This enables us to further rewrite \mathbf{M}_i :

$$\mathbf{M}_{i} = \left(\mathbf{L}\left(\mathbf{U}d(\mathbf{v})\mathbf{U}^{\top} + \mathbf{U}\mathbf{U}^{\top}s_{i}\right)\mathbf{L}^{\top}\right)^{-1}$$

$$= \left(\mathbf{L}\mathbf{U}d(\mathbf{v} + s_{i})\mathbf{U}^{\top}\mathbf{L}^{\top}\right)^{-1}$$

$$= \left(\mathbf{L}^{-1}\right)^{\top}\mathbf{U}d\left((\mathbf{v} + s_{i})^{-1}\right)\mathbf{U}^{\top}\mathbf{L}^{-1}. \quad \Box$$
(C.3)

Proof Determinant

Using the general properties of the determinant and the identity that $UU^{T} = I$:

$$\det(\mathbf{M}_{i}) = \det((\mathbf{L}^{-1})^{\top} \mathbf{U} d((\mathbf{v} + s_{i})^{-1}) \mathbf{U}^{\top} \mathbf{L}^{-1})$$

$$= \det((\mathbf{L}^{-1})^{\top}) \det(\mathbf{U}) \det(d((\mathbf{v} + s_{i})^{-1})) \det(\mathbf{U}^{\top}) \det(\mathbf{L}^{-1})$$

$$= \det(\mathbf{U} \mathbf{U}^{\top}) \det((\mathbf{L}^{-1})^{\top}) \det(d((\mathbf{v} + s_{i})^{-1}))$$

$$= \det(\mathbf{C})^{-1} \prod_{k=1}^{K} (v_{k} + s_{i})^{-1}. \quad \Box$$
(C.4)

Endnotes

- ¹ "Small baskets, large stores—how shopping behaviour is changing," dunnhumby, March 20, 2017. (https://www.dunnhumby.com/resources/reports/small-baskets-large-stores)
- ² "Can grocery stores embrace change and technology?," Forbes, May 28, 2019 (https://www.forbes.com/sites/lanabandoim/2019/05/28/can-grocery-stores-embrace-change-and-technology).
- ³ "Amazon's new weapon to crush competition: \$1 items delivered for free—by tomorrow," Vox, October 14, 2019 (https://www.vox.com/recode/2019/10/14/20906728/amazon-prime-low-price-products-add-on-one-day-delivery).
- ⁴ "Using purchase history to identify customer 'projects'," Wharton Customer Analytics (https://wca.wharton.upenn.edu/research/using -purchase-history-to-identify-customer-projects/).
- ⁵ In the marketing literature, the softmax function is better known as the multinomial logit *function*, but we want to avoid confusion with the equivalent named multinomial logit *model*.
- ⁶ In our notation, we implicitly condition on other exogenous information that is available, that is, the parameters describing the prior distribution $p(\Omega)$ and the explanatory variables x and w.
- ⁷Our code is available as a Python package on https://brunojacobs.com.

- ⁸ We are grateful to Wharton Customer Analytics (WCA) for setting up the research opportunity that has connected us to this retailer.
- ⁹We emphasize that the product taxonomy is only used to aggregate infrequent products in the data. More specifically, the product taxonomy is not used in the model and the identification of motivations does not rely on the product taxonomy.
- ¹⁰The Markov blanket for a parameter is defined as its parents, children, and the co-parents of its children in the directed acyclical graph (DAG) representation of the model (Pearl 2009).

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