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Analyzing market basket data through sparse multivariate logit models

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Abstract

Using multivariate logit models, we analyze purchases of product categories made by individual households. We introduce a sparse multivariate logit model that considers only a subset of all two-way interactions. A combined forward and backward selection procedure based on a cross-validated performance measure excludes about 74 % of the possible two-way interactions. We also specify random coefficient versions of both the non-sparse and the sparse model. The fact that the random coefficient models lead to better values of the Bayesian information criterion demonstrates the importance of latent heterogeneity. The random coefficients sparse model attains the best statistical performance if we consider model complexity and ofers a better interpretability. We investigate the cross-purchase efects of household segments derived from this random coefficient model. As additional interpretation aid we cluster categories and category pairs by integer programming. We demonstrate what the best performing sparse model implies for cross-selling by product recommendations and store layout. The sparse model leads to managerial implications with respect to the efects of advertising in local newspapers and fyers that are as a rule close to those implied by its non-sparse counterpart.

Keywords Retailing · Multicategory choice · Market basket analysis · Multivariate logit model

Introduction

Multicategory choice models like the frequently applied multivariate logit (MVL) model analyze pick-any choices characterized by the fact that households may purchase multiple product categories on the same occasion (Hruschka et al. [1999](#page-14-0); Russell and Petersen [2000;](#page-14-1) Boztuğ and Hildebrandt [2008](#page-14-2); Boztuğ and Reutterer [2008;](#page-14-3) Dippold and Hruschka [2013;](#page-14-4) Aurier and Mejia [2014;](#page-14-5) Richards et al. [2018](#page-14-6); Solnet et al. [2016](#page-15-0); Hruschka [2024\)](#page-14-7). The MVL model allows for two-way interactions between purchases of diferent product categories. A positive two-way interaction exists if the purchase of category j_1 increases the purchase probability of another category j_2 . For example, the purchase of snacks could increase the purchase probability of beverages. In a negative two-way interaction, on the other hand, the purchase of category j_1 decreases the purchase probability of another category j_2 (e.g., the purchase of cold cereal could decrease the purchase probability of beer).

As a rule, the MVL model includes all two-way interactions between categories. For our data set with 31 categories, the number of all two-way interactions amounts to 465. Such a high number makes interpretation difficult. The use of sparse MVL (SVML) models in which purchases depend only on a subset of interactions improves interpretability. Despite this advantage of SMVL models, to our knowledge only few relevant publications exist. Hruschka et al. ([1999](#page-14-0)) start from the MVL model with all two-way interactions applying a greedy stepwise backward elimination that stops if only significant coefficients remain. Dippold and Hruschka ([2013](#page-14-4)) determine signifcant interactions by Bayesian variable selection techniques. The approach of Boztuğ and Reutterer [\(2008\)](#page-14-3) consists of two steps. In the frst step, these authors cluster market baskets by an online K-means algorithm. In the second step, they estimate one MVL model for the categories assigned to a cluster. This approach only allows two-way interactions between the categories of a cluster and sets interactions with categories of other clusters to zero.

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The multivariate probit (MVP) model represents an alternative multicategory choice model that is quite often applied to market basket data (Chib et al. [2002;](#page-14-8) Duvvuri et al. [2007](#page-14-9); Manchanda et al. [1999;](#page-14-10) Hruschka [2017](#page-14-11); Aurier and Mejia [2014\)](#page-14-5). In the MVL model the purchase probability of a category may be afected by current purchases of other categories. The MVP model does not include such current effects, it reproduces interdependences between categories by correlations of error terms. Error terms are assumed to follow a multivariate normal distribution whose parameters are constant across time. The fact that the MVP model puts more weight on joint non-purchases of category pairs, because they are much more frequent than joint purchases, is a related critical issue (Seetharaman et al. [2005](#page-14-12)). On the other hand, the MVL model takes only joint purchases into account. Which assumption on pairwise category interdependences leads to a better statistical performance, remains an empirical question.

For the MVL model selection of interactions comes down to straightforward selection of certain coefficients. The selection of pairwise correlations for the MVP model turns out to be more involved. Appropriate methods for the MVP model typically determine a spare inverse correlation matrix (Talhouk et al. [2012](#page-15-1)) whose elements are harder to interpret than elements of a correlation matrix.

In our MVL models we not only consider two-way interactions, we allow for three-way interactions as well. In a three-way interaction the joint purchase of two categories j_1 and j_2 increases (decreases) the probability of another category j_3 . For the MVL and the SMVL models, expressions ([4\)](#page-3-0) and ([7](#page-3-1)) show that the latent variable of any category linearly depends on purchases of all the other and of selected other categories or pairs of other categories, respectively.

The MVP model, however, does not include three-way interaction terms. Its latent variables have the structure of a linear seemingly unrelated regression (SUR) model (Zellner [1971\)](#page-15-2). Each expected conditional latent variable of a category in the MVP model linearly depends on the product of the inverse error correlation matrix with the row and column indicating category j_1 eliminated and the vector of errors for the latent variables of the remaining categories (Albert and Chib [1993](#page-14-13); Chib and Greenberg [1998\)](#page-14-14).

In the following we discuss several machine learning methods that have recently been applied to market basket data, namely topic models (TMs), the restricted Boltzmann machine (RBM), the deep belief net (DBN), the skip-gram model (SGM) and a deep neural net with bottleneck layers (DNNBL). For these machine learning methods, the number of latent variables is usually lower than the number of categories. Whereas the MNL and MNP provide parameters $(i.e., coefficients or correlations)$ directly measuring interactions, machine learning techniques require additional computations after estimation. Of course, this property of most

machine prevents selection of interaction terms as part of the estimation process.

The discrete latent variables of TMs are called topics. TMs comprise two multinomial distributions, topic proportions of categories and topic proportions of baskets (Hruschka [2014b;](#page-14-15) Jacobs et al. [2016\)](#page-14-16).

The restricted Boltzmann Machine (RBM) includes twoway interactions between latent variables and categories (Hruschka [2014a\)](#page-14-17). Deep belief nets (DBN) stack several RBMs. Each higher level RBM processes the latent variables from the level immediately below (Hruschka [2014a\)](#page-14-17).

The DBN also includes a further layer DBN connecting latent variables of the last layer to observed purchases of each category by a binary logistic function. For the TMs and the RBM two-way interaction measures between categories can be computed after estimation as dot product of two vectors each holding topic proportions and interaction coefficients with respect to latent variables, respectively.

Gabel et al. ([2019](#page-14-18)) adapt the SGM, which was originally developed for natural language processing, to market basket analysis. The other models mentioned so far analyze either the probability of a whole market basket or the purchase probability of each category conditional on the remaining purchased categories. The SGM, on the other hand, considers cross-occurrences of (ordered) category pairs. Therefore, the number of equations to be estimated increases quadratically with the number of purchases categories contained in a basket. The probability of a cross-occurrence depends on a cross-occurrence score, specifed as dot product of the estimated latent variables for the two categories. Gabel et al. [\(2019](#page-14-18)) demonstrate that cross-occurrence scores are strongly related to the error correlations of a MVP model.

The SGM represents an exploratory approach, which is especially appropriate if a large number of products should be analyzed. Gabel et al. ([2019\)](#page-14-18) suggest to use the SGM to decide which categories or products should be considered in a multicategory choice model like the MVL or MVP. Like the other machine learning methods discussed the estimation does not select interactions or cross-occurrences.

Gabel and Timoshenko [\(2022](#page-14-19)) develop a DNNBL for market basket analysis. These authors obtain summaries of purchase histories (i.e., market baskets of individual households across several periods) by applying several linear time series flters transformed by a neural activation function. Bottleneck layers capture cross-product relationships by compressing these summaries, average purchase frequencies and current coupons for all products. Outputs of bottleneck layers are projections of the compressed data back to the higher original dimension. Conditional purchase probabilities of each product result from plugging product-specifc inputs and outputs of bottleneck layers into a binary logit function.

Our paper contributes over the extant literature as follows. Estimation of the SVML model consists of a forward selection stage and a backward elimination stage. The frst stage selects in each step the predictor (e.g., a marketing variable, a two-way interaction, a three-way interaction) with the greatest performance improvement. The steps of the second stage look at reductions of the cross-validated performance measure. Cross-validation makes selection of predictors more robust as opposed to greedy backward elimination. To account for the heterogeneity of households, we extend the MVL and the SVML models to random coefficient models (abbreviated as RC-MVL and RC-SVML). To further improve interpretability, we cluster categories and pairs of categories being part of a three-way interaction based on estimation results in contrast to Boztuğ and Reutterer ([2008\)](#page-14-3) who form clusters beforehand.

In "[Models](#page-2-0)" section we specify the MVL and SMVL as well as their random coefficient versions. We also deal with estimation and performance evaluation of these models. In addition we present fnite mixture versions of the MVL and SMVL models. In "[Cross-purchase efects of house](#page-5-0)[hold segments"](#page-5-0) section we explain how we investigate the cross-purchase efects for household segments derived from the random coefficient version. "Clustering categories and [category pairs"](#page-7-0) section introduces clustering of categories and category pairs being part of three-way interactions based on estimation results as interpretation aid for sparse models. In "[Data"](#page-8-0) section we characterize the data set by means of descriptive statistics in "[Data](#page-8-0)" section. "[Estimation results"](#page-9-0) section presents estimation results. "[Obtained cross-pur](#page-10-0)[chase efects of household segments](#page-10-0)" and ["Obtained clusters](#page-11-0) [of categories and category pairs](#page-11-0)" sections discuss obtained segment-specific cross-purchase effects and category clusters, respectively. In "[Managerial implications"](#page-12-0) section we demonstrate what sparse models imply for cross-selling by product recommendations and store layout. We also investigate whether implications with respect to category-specifc advertising by local newspapers and fyers difer between sparse and non-sparse models. In "[Conclusion"](#page-13-0) section we summarize results and also discuss other applications and extensions of our approach in future research.

Models

J column vector *ymt* denotes market basket *t* of household *m* and consists of binary purchase indicators (*J* symbolizes the number of product categories). If household *m* purchases category *j* on purchase occasion *t*, the respective element y_{jmt} equals one. Vector x_{mt} consists of regressors relevant for the market basket *t* of household *m*. In our study, these regressors consist of category loyalties and the categoryspecifc marketing variable feature, i.e., advertising in local newspapers and fyers. Due to multicollinearity leading to many coefficients with implausible signs we decided not to add category-specifc prices as regressors.

We compute the loyalty of household *m* for category *j* in market basket *t* in analogy to exponentially smoothed brand loyalties (Guadagni and Little [1983](#page-14-20)):

$$
loy_{jmt} = \alpha y_{jmt-1} + (1 - \alpha) \, loy_{jmt-1} \tag{1}
$$

 $0 \le \alpha \le 1$ denotes the smoothing constant. The binary purchase incidence *yjmt*[−]1 equals one, if household *m* purchases category *j* on the previous purchase occasion *t* − 1. The current category loyalty depends on the previous purchase incidence *yjmt*[−]1 and the previous loyalty *loyjmt*[−]1. In a manner similar to the brand loyalty of Guadagni and Little ([1983\)](#page-14-20) we set initial values \log_{im0} equal to the relative purchase frequency of the respective category *j* across all households and shopping visits $(t = 1$ denotes the first shopping visit). The lower the smoothing constant α is, the less the loyalty variable refects fuctuating purchases.

We use the Bayesian information (BIC) to evaluate models (Cameron and Trivedi [2007\)](#page-14-21):

$$
BIC = -2 LPL + np \ln(N) \tag{2}
$$

LPL denotes the total log pseudo-likelihood, *np* the number of parameters and *N* the number of observations. We explain the computation of the LPL for each model in "[Multivariate](#page-2-1) [logit model"](#page-2-1)-"Random coefficient and finite mixture mod[els](#page-4-0)" sections. The BIC considers model complexity, i.e., it penalizes models with respect to the number of parameters. Models attaining low BIC values are to be preferred.

Multivariate logit model

Extending the expression for the MVL model without regressors (also known as auto-logistic model) given in Besag [\(1972\)](#page-14-22) we defne the probability of market basket *ymt* conditional on regressors x_{mt} as follows:

$$
\exp(y'_{mt}a + x'_{mt}By_{mt} + 1/2y'_{tm}Dy_{mt})/C
$$

with
$$
C = \sum_{\psi \in \{0,1\}^J} \exp(\psi'a + x'_{mt}B\psi + 1/2\psi'D\psi)
$$
 (3)

Expression ([3](#page-2-2)) shows that computation of this probability requires division by the normalization constant *C* that is obtained by summing over all possible market baskets represented by different binary vectors ψ . Coefficients contained in the (J, J) matrix D measure two-way interactions between categories. As a two-way interaction of a category with itself does not make sense, all diagonal elements of *D* are zero. Off-diagonal elements are symmetric, i.e., $d_{i1,i2} = d_{i2,i1}$. Column vector *a* consists of *J* category constants. The (K, J) matrix *B* holds the effect of *K* regressors on purchase

probabilities. The MVL model has been applied to market basket data by Russell and Petersen ([2000](#page-14-1)) building upon earlier publications in statistics (Cox [1972](#page-14-23); Besag [1974\)](#page-14-24).

We can write the purchase probability of category *j* in market basket *t* of household *m* conditional on purchases of the other categories collected in vector *y*−*jtm*, the categoryspecifc loyalty *loyjmt* and the category-specifc marketing variable *mvar*_{it} as:

$$
P(y_{jmt} = 1 | y_{-jmt}, x_{mt}) = \varphi(Z_{jmt})
$$

\n
$$
Z_{jmt} = a_j + b_j l \omega y_{jmt} + c_j m \nu a r_{jt} + \sum_{l \neq j} d_{j,l} y_{lmt}
$$
\n(4)

 φ (*Z*) denotes the binomial logistic function $1/(1 + exp(-Z))$. *Zjmt* can be interpreted as latent variable referring to category *j* and market basket *t* of household *m*.

Maximum likelihood estimation of the MVL model requires in each iteration the computation of the normalization constant (see expression (3) (3)). For the 31 categories in our study, we would have to sum over more than 2.14×10^9 possible market baskets. Maximum pseudo-likelihood (MPL) estimation (Bel et al. 2018) offers a viable alternative maximizing the log pseudo-likelihood *LPL* across households, market baskets and categories:

$$
LPL = \sum_{m=1}^{M} \sum_{t=1}^{T_m} \sum_{j=1}^{J} \log(\tilde{P}_{jmt})
$$
\n(5)

Tm symbolizes the number of market baskets of household *m*, \tilde{P}_{jmt} the pseudo-probability of a (non) purchase of category *j* in market basket *t* of household *m*. Summing logarithmic pseudo-probabilities across *J* product categories makes MPL estimation feasible as it replaces the summation across all possible baskets, which would be necessary in maximum likelihood estimation. The pseudo-probability \tilde{P}_{jmt} can be written as:

$$
\tilde{P}_{jmt} = P(y_{jmt} = 1|y_{-jmt}, x_{mt})^{y_{jmt}}
$$
\n
$$
(1 - P(y_{jmt} = 1|y_{-jmt}, x_{mt}))^{1 - y_{jmt}}
$$
\n(6)

Expression [\(4](#page-3-0)) shows how to compute the conditional probability $P(y_{jmt} = 1|y_{-jmt}, x_{mt})$ for the MVL model. y_{jmt} denotes the binary purchase indicator, which is set to one if basket *t* of household *m* contains category *j*. One can see from Eq. [\(6](#page-3-2)) that its frst part is relevant if category *j* is purchased and its second part if category *j* is not purchased. Briefy, LPL estimation looks at *J* diferent binomial logit models representing conditional probabilities.

Sparse multivariate logit model

Like the MVL we estimate the SMVL by maximizing the LPL using *J* binomial logit models. The SMVL difers from the MVL by the specifcation of the conditional probabilities that:

- may exclude the marketing variable or the category loyalty of the respective category.
- as a rule includes a subset of the purchases of other categories only.
- may include joint purchases of pairs of other categories.

Consequently, we write the conditional purchase probability of category *j* in market basket *t* of household *m* for the SMVL model as:

$$
P(y_{jmt} = 1 | y_{-jmt}, x_{mt}) = \varphi(Z_{jmt})
$$
\n(7)

$$
Z_{jmt} = a_j + u_j^1 b_j l o y_{jmt} + u_j^2 c_j m v a r_{jt}
$$

+
$$
\sum_{k \in J_j^1} d_{j,k} y_{lmt} + \sum_{(I1,I2) \in J_j^2} e_{j,I1,I2} y_{I1mt} y_{I2mt}
$$

 $\log_{jmt} (mvar_{jt})$ is exluded if the binary variable $u_j^1 j(u_j^2)$ equals 0. Two-way interactions of category *j* with a category *k* are included if *k* belongs to set \mathbb{J}^1_j that must not contain category *j*. Sparsity mainly results from excluding purchases of many other categories. Three-way interactions of category *j* with categories *l*1 and *l*2 are included if the pair (*l*1, *l*2) belongs to set J_j^2 that must not contain pairs having category *j* as one of their two elements.

For each of *J* categories we determine optimal values of two hyperparameters based on a fve-fold cross-validation. The frst hyperparameter has 19 values, i.e., the integer number of coefficients $(2, 3, \ldots, 20)$. The second hyperparameter has two values that indicate whether three-way interaction may be included or not. We perform a grid search to select the hyperparameter mix from $38 = 19 \times 2$ combinations. This grid search provides the two binary variables u_j^1 , u_j^1 and the two sets J_j^1 , J_j^2 of expression [\(7](#page-3-1)). Please note that each of these two sets may be empty meaning that two-way interactions and three-way interactions are excluded, respectively.

The Multivariate Adaptive Regression Splines (MARS) method (Friedman [1991](#page-14-26); Kuhn and Johnson [2013](#page-14-27)) serves to search specifications with log loss ll_j of category *j* as performance measure:

$$
ll_{j} = \sum_{m=1}^{M} \sum_{t=1}^{T_{m}} -\log(\tilde{P}_{jmt})/N
$$

\n
$$
\tilde{P}_{jmt} = P(y_{jmt} = 1|y_{-jmt}, x_{mt})^{y_{jmt}}
$$

\n
$$
(1 - P(y_{jmt} = 1|y_{-jmt}, x_{mt}))^{1 - y_{jmt}}
$$

\n
$$
N = \sum_{m=1}^{M} T_{m}
$$
\n(8)

Log losses are related to the log pseudo-likelihood of expression ([5\)](#page-3-3) as follows:

$$
LPL = -N \sum_{j=1}^{J} ll_j
$$
\n(9)

MARS builds additive models based on the set of predictor variables (here: category loyalty, marketing variable, two-way and three-way interactions). In the frst stage the algorithm operates recursively, incorporating at each step the predictor variables leading to the greatest performance improvement. The second stage consists of a backwards elimination routine that looks at reductions of the crossvalidated performance measure. Optimal values of hyperparameters are taken from the minimum mean out-of-fold performance measure. MARS then rebuilds the corresponding model using all the data.

Please be aware that we do not use splines, as all predictors are linearly related to the latent variable Z_{imt} in expression ([7](#page-3-1)). Most of the considered predictors are binary. MARS is known to perform well for binary predictors for which it was not originally developed (Ruczinski et al. [2003](#page-14-28)).

Random coefficient and finite mixture models

To take latent heterogeneity of households into account we extend the MVL and SMVL models to versions with random coefficients. Each random coefficient model consists of *J* different random coefficient binomial logit models, i.e., one for each product category. To simplify matters, we speak of a random coefficient multivariate logit model in the following to denote such a set of models.

We estimate random coefficient models by maximum simulated pseudo-likelihood using Halton draws and normal mixing distributions for category constants and random coefficients of predictors (Train [2003](#page-15-3)). Additional suffixes *r* symbolize the r-th draw of a category constants or a coefficient from the mixing distribution. For the random coefficient multivariate logit (RC-MVL) model we specify the r-th draw of latent variable *Zjmtr* of category *j* in market basket *t* of household *m* as:

$$
Z_{j m t r} = a_{j r} + b_{j r} l o y_{j m t} + c_{j r} m v a r_{j t} + \sum_{l \neq j} d_{j, l, r} y_{l m t}
$$
(10)

The random coefficient sparse multivariate (RC-SMVL) model encompasses the predictors selected by the SVML model; it difers from the former by considering random draws of parameters. The *r*-th draw of latent variable *Zjmtr* of category *j* in market basket *t* of household *m* is:

$$
Z_{jmlr} = a_{jr} + u_j^1 b_{jr} \log_{jmt} + u_j^2 c_{jr} \max_{j} t + \sum_{k \in \mathbb{J}_j^1} d_{j,k,r} y_{lmt} + \sum_{(l1,l2) \in \mathbb{J}_j^2} e_{j,l1,l2,r} y_{l1mt} y_{l2mt}
$$
(11)

For each random coefficient model the conditional purchase probability of category *j* in market basket *t* of household *m* based on the r-th draw is:

$$
P_r(y_{jmt} = 1|y_{-jmt}, x_{mt}) = \varphi(Z_{jmtr})
$$
\n(12)

The corresponding pseudo-probability \tilde{P}_{intr} can be written as:

$$
\tilde{P}_{jmtr} = P_r(y_{jmt} = 1|y_{-jmt}, x_{mt})^{y_{jmt}}
$$
\n
$$
(1 - P_r(y_{jmt} = 1|y_{-jmt}, x_{mt}))^{1 - y_{jmt}}
$$
\n(13)

We consider that as a rule we observe several market baskets for a household. Both for the RC-MVL and the RC-SMVL model we therefore compute the pseudo-likelihood *PLjm* for category *j* and household *m* over T_m baskets as average across *R* samples:

$$
PL_{jm} = (1/R) \sum_{r=1}^{R} \prod_{t=1}^{T_m} \tilde{P}_{jmtr}
$$
 (14)

Summing across households and categories we obtain the total log pseudo-likelihood of a random coefficient model:

$$
LPL = \sum_{m=1}^{M} \sum_{j=1}^{J} \log PL_{jm}
$$
 (15)

We now present fnite mixture extensions of these models for the readers' beneft though we do not investigate these models in more detail. Coefficients differ between *S* household segments with $s = 1, \ldots, S$. We specify segment-specific latent variables for the MVL and the SMVL models as:

$$
Z_{jmts} = a_{js} + b_{js} \log_{jmt} + c_{js} m \sqrt{ar_{jt}} + \sum_{l \neq j} d_{j,l,s} \sqrt{v_{lmt}}
$$
 (16)

$$
Z_{jmts} = a_{js} + u_j^1 b_{js} \log_{jmt} + u_j^2 c_{js} mvar_{jt} + \sum_{k \in J_j^1} d_{j,k,s} y_{lmt} + \sum_{(l1,l2) \in J_j^2} e_{j,l1,l2,s} y_{l1mt} y_{l2mt}
$$
 (17)

The total log pseudo-likelihood for the fnite mixture extensions results from expressions (6) (6) and (5) (5) with the following conditional purchase probability of category *j* in market basket *t* of household *m*:

$$
P(y_{jmt} = 1 | y_{-jmt}, x_{mt}) = \sum_{s=1}^{S} f_{sm} \varphi(Z_{jmts})
$$
\n(18)

Fig. 1 Cluster-Specifc Directed Graphs. Explanation: Directed edges indicate that a category or category pair afects another category. Categories and category pairs are identifed by the numbers given in Table [15](#page-11-1). Examples for cluster 4: frozen pizza (11) affects frozen dinners (10) , cold cereal (17) affects milk (6) and vice versa, the category pair cold cereal (6) and milk (17) affects yoghurt (31)

Table 1 Product categories and abbreviations

fsm is the probability that household *m* belongs to segment *s* with $\sum_{s=1}^{S} f_{sm} = 1.0$.

Cross‑purchase efects of household segments

We want to investigate how households difer in terms of their cross-purchase behavior implied by a random coefficient model. To this end we determine household-specific coefficients in the first step (Train [2003;](#page-15-3) Greene [2003\)](#page-14-29).

For each random coefficient we draw *R* random samples from the normal distribution using means and standard deviations that were estimated before. From expression ([13](#page-4-1)) we obtain the log pseudo-likelihood *PLjmr* of draw *r* for category *j* and household *m* over T_m baskets as:

Table 3 Relative pairwise frequencies

Shows the 20 highest relative pairwise frequencies

Table 4 Average category

Table 4 Average category lovalties	milk	0.359	carbbey	0.307	saltsnck	0.274	coldcer	0.218
	yogurt	0.161	soup	0.149	spagsauc	0.142	toitisu	0.133
	margbutr	0.119	paptowl	0.109	coffee	0.103	laundet	0.092
	fzpizza	0.084	mayo	0.084	hotdog	0.081	mustketc	0.081
	fzdin	0.070	factiss	0.065	peanbutr	0.062	beer	0.058
	toothpa	0.046	shamp	0.041	deod	0.032	cigets	0.026
	hhclean	0.023	diapers	0.015	blades	0.014	toothbr	0.010
	sugarsub	0.009	photo	0.004	razors	0.001		
Table 5 Average features	fzdin	0.187		0.179	carbbev	0.175	fzpizza	0.174
			yogurt					
	diapers	0.171	spagsauc	0.169	saltsnck	0.154	coldcer	0.151
	peanbutr	0.133	margbutr	0.130	milk	0.129	coffee	0.124
	factiss	0.119	soup	0.112	laundet	0.106	mayo	0.100
	toitisu	0.095	hotdog	0.094	shamp	0.094	razors	0.093

toothpa 0.089 deod 0.083 paptowl 0.067 beer 0.061 hhclean 0.041 mustketc 0.041 blades 0.040 photo 0.039

toothbr 0.017 sugarsub 0.008 cigets 0.000

Table 6 Model evaluation results

Model	Pseudo log-likelihood	Number of parameters	BIC
Without loyalties and features			
MVL	$-224,868$	496	454,740
SMVL	$-226,047$	267	454,788
With loyalties and features			
MVL	$-181,863$	558	369,356
SMVL	$-182,877$	234	368,115
RC-MVL	$-177,151$	589	360,244
RC-SMVL	$-178,644$	265	359,962

24,074 observations; values rounded to the nearest integer

$$
\log PL_{jmr} = \sum_{t=1}^{T_m} \log \tilde{P}_{jmr} \tag{19}
$$

Each household-specific coefficient corresponds to a weighted average of its draws. These weights $w_{mr} = \exp(\log PL_{jmr}) / \sum_{r=1}^{R} \exp(\log PL_{jmr})$ indicate the relative importance of random draw *r* for household *m*.

In the second step we apply K-means to the householdspecific coefficients to obtain household segments. Each segment is characterized by its centroid, i.e., the coeffcients averaged across all households allocated to this segment.

Now we are able to compute segment-specifc crosspurchase efects for a segment *s* using its averaged coefficients. We measure the cross-purchase effects of category *j* on category j' of category by the difference of purchase probabilities of category j' conditional on a high and a low purchase probability of category *j*. Please note that crosspurchase effects are as a rule not symmetric, i.e., the effect of category j on category j' differs from the effect of category *j* ′ on category *j*.

As expressions ([4](#page-3-0)) and ([7\)](#page-3-1) give conditional probabilities only we have to determine unconditional purchase **Table 7** RC-SMVL model: equations of latent variables $Z_{imt}(1)$

Equations include fixed coefficients and mean category constants with a significance level less equal 0.001

Equations include fixed coefficients and mean category constants with a significance level less equal 0.001

probabilities. We simulate purchases by iterated Gibbs-sampling from the appropriate conditional distributions (Besag [2004](#page-14-30)) using segment-specific coefficients. We estimate the unconditional purchase probability of a category by its marginal relative frequency across the simulated purchases.

Clustering categories and category pairs

As interpretation aid for of the SVML or RC-SVML models we determine clusters of categories and category pairs being part of three-way interactions. This clustering works on a graph whose nodes represent categories and category pairs (see expressions (7) (7) and (11) (11)). Nodes of the graph link each

Table 10 standard constants

Equations include fixed coefficients and mean category constants with a significance level less equal 0.001

Shows standard deviations with a signifcance level less equal 0.001

category *j* to each of the other categories contained in \mathbb{J}^1_j and to each three-way interaction contained in \mathbb{J}^2_j . The graph has no node for a category *j* if both J_j^1 and J_j^2 are empty and category *j* is contained neither in \mathbb{J}_k^1 nor in \mathbb{J}_k^2 for each of the other categories $k \neq j$. We say that such a category *j* is isolated.

We measure the quality of a clustering *ℂ* with *C* clusters by its modularity (Brandes et al. [2008](#page-14-31)):

$$
Q(\mathbb{C}) = \sum_{C \in \mathbb{C}} \left[\frac{m_c}{m} - \left(\frac{\sum_{v \in C} n(v)}{2m} \right)^2 \right] \tag{20}
$$

 m_C symbolizes the number of links that are assigned to cluster *C*, *m* the total number of links, $n(v)$ the number of links with node *v*.

Modularity refects two conficting objectives (Brandes et al. [2008](#page-14-31)). Its frst term becomes higher for a low number of clusters, each with many links contained. On the other hand, its second term gets lower for a high number of clusters each with a small number of links. Modularity measures the diference between the total fraction of links that fall within clusters and the expected fraction if links were placed at random considering the number of links to nodes (Porter et al. [2009](#page-14-32)). To obtain clusters we maximize modularity by integer programming (Brandes et al. [2008](#page-14-31)). In contrast to heuristic search algorithms, integer programming is guaranteed to determine the global optimum and provides both the optimal number of clusters and the optimal assignment of links to these clusters.

Empirical study

Data

Our data refer to 24,047 shopping visits made by a random sample of 1500 households to one specifc grocery store over a one-year period. For each shopping visit, we compose a market basket from the IRI data set Bronnenberg et al. [\(2008](#page-14-33)). We represent a market basket by a binary vector whose elements indicate whether a household purchases each of 31 product categories (see Table [1\)](#page-5-1). The average number of shopping visits per household amounts to 16.031, its standard deviation to 13.464. The average basket size (i.e., number of purchased categories) is 3.852, its standard deviation 2.654.

Table [2](#page-5-2) shows relative marginal purchase frequencies for the 31 categories. Milk (razors) is the category most (least) frequently purchased. Table [3](#page-6-0) gives the highest 20 pairwise relative frequencies. Carbonated beverages and milk are the two categories most frequently purchased together, followed by carbonated beverages and salty snacks.

Table [4](#page-6-1) contains the average loyalty across all market baskets for each category with a smoothing constant $\alpha = 0.1$, which puts most weight on the loyalty of the previous week. This value of the smoothing constant leads to the best performing MVL model with category loyalty according to a grid search over [0.1, 0.2, 0.3, …, 0.9]. Given such a value,

previous purchases are strongly smoothed. Milk attains the highest category loyalty, followed by carbonated beverages and salty snacks. Average category loyalties are remarkably similar to relative marginal purchase frequencies.

We measure features as weekly market share-weighted averages of UPC level variables in the respective category. Consequently, features take values between zero and one. Table [5](#page-6-2) shows average values of features for each category. We obtain the highest (lowest) average feature value for frozen dinners (cigarettes).

Table 12 Segment-specifc cross-purchase efects (1)

Shows cross-purchase efects of the left category on the right category greater equal 0.0030

Estimation results

Table [6](#page-6-3) contains BIC values of the six investigated models. Adding loyalty and features as predictors improves BIC values both for the MVL and the SMVL model.

For both the RC-MVL and the RC-SMVL models standard deviations of predictors' random coefficients are as a rule not signifcantly diferent from zero. Therefore, we use fxed coefficients for loyalty, feature, 2-way and 3-way interactions, only category constants are random. These random coefficient models lead to clearly lower BIC values though they only have 31 parameters more. Overall, the RC-SMVL with predictors outperforms the other investigated models. From now on we only discuss the RC-MVL and RC- SMVL models as their performance is better than that of related models without random coefficients.

Tables [7,](#page-7-1) [8](#page-7-2) and [9](#page-8-1) contain the equations of the 31 category-specifc latent variables *Zjmt* for the RC-SMVL model. These equations only include mean category constants and fixed coefficients that are significant (to simplify terminology, we only write that a mean category constant or a fxed

Shows cross-purchase efects of the left category on the right category greater equal 0.0030

Table 14 Additional segment-specifc cross-purchase efects

Segment 2 vs. Segment 1					
toitisu	paptowl	0.0046	coldcer	margbutr	0.0040
yogurt	coldcer	0.0036	coldcer	spagsauc	0.0030
Segment 3 vs. Segment 2					
yogurt	milk	0.0094	coldcer	yogurt	0.0056
coldcer	soup	0.0038	soup	yogurt	0.0036
mustketc	mayo	0.0030			
Segment 4 vs. Segment 2					
mustketc	mayo	0.0032	spagsauc	carbbey	0.0030
yogurt	milk	0.0030			
Segment 5 vs. Segment 2					
spagsauc	carbbey	0.0036			
Segment 6 sv. Segment 3					
coldcer	spagsauc	0.0034			
Segment 7 vs. Segment 6					
soup	spagsauc	0.0036	spagsauc	soup	0.0034
spagsauc	carbbey	0.0032			
coldcer	soup	0.0032			

Shows cross-purchase effects of the first segment additional to those of the second segment greater equal 0.0030

coefficients is significant if significant at a confidence level of 0.001).

The majority of equations include both loyalty and feature. Their coefficients are positive, i.e., higher values of these predictors increase the conditional purchase probability. Exceptions are the equations for blades, diapers, margarine & butter, mayonnaise, mustard & ketchup, shampoo and tooth paste, which include only feature and the equation for cigarettes which include only loyalty. Equations for razors, sugar substitutes and tooth brush exclude both loyalty and feature.

According to Table [10](#page-8-2) standard deviations of constants are signifcant for all categories except blades. Both the size of standard deviations of category constants and the superior statistical performance of the RC-SMVL model (see Table [6\)](#page-6-3) underline that taking the latent heterogeneity of households into account is important.

The total number of signifcant two-way interactions amounts to 120. These two-way interactions are all positive, indicating that the categories involved are purchase complements (i.e., purchase of category j_1 increases the conditional purchase probability of category j_2). Many food/drink categories are often afected only by other food/drink categories (frozen dinners, frozen pizza, frankfurters & hotdog, mayonnaise, mustard & ketchup, milk, peanut butter, salty snacks, sugar substitutes, yogurt). In an analogous way, several non-food categories are afected only by other non-food categories (blades, deodorant, tooth brush).

Three-way interactions are as a rule positive, i.e., a joint purchase of categories j_1 and j_2 (e.g., razors and shampoo) increases the conditional probability of the affected category j_3 (e.g., blades). We obtain only one negative threeway interaction, namely for razors with the two categories blades and soup. A joint purchase of blades and soup lowers the conditional purchase probability of razors.

Table [11](#page-9-1) gives the number of interactions for each category with other categories and category pairs. This table also contains the number of categories afected by two-way and three-way interactions. Four categories are afected neither by purchases of other categories nor by purchases of category pairs (beer & ale, cigarettes, diapers, photographic supplies). For the remaining 27 categories, the number of such interactions varies between one and ten (e.g., 10 for soup, 9 for cold cereal, 8 for salty snacks, spaghetti sauce and toilet tissue).

Obtained cross‑purchase efects of household segments

To determine segment-specifc cross-purchase efects for the RC-SVML model we apply the procedure explained in "[Cross-purchase efects of household segments](#page-5-0)" section. The elbow criterion suggests a solution with eight segments

*Indicates a category pair which is part of a three-way interaction

whose shares amount to 0.30, 0.19, 0.131, 0.105, 0.101, 0.071, 0.071, and 0.017, respectively. We ignore segment eight because of its low share in the following.

We obtain positive cross-purchase effects only. Therefore, we classify the involved categories as purchase complements in accordance with Betancourt and Gautschi ([1990\)](#page-14-34), who consider two categories as purchase complements if they are purchased jointly more frequently than expected under stochastic independence.

Cross-purchase effects greater equal 0.003 are listed in Tables [12](#page-9-2) and [13](#page-10-1). The number of these cross-purchase efects difers between segments (e.g., seven for segment 1 versus sixteen for segment 7).

The seven cross-purchase efects of segment 1 arise in the other segments as well. Nonetheless, categories involved in cross-purchase efects are heterogenous across segments. For selected segment pairs Table [14](#page-10-2) shows cross-purchase efects turning out for a segment in addition to those relevant for the other segment. Interestingly, these additional crosspurchase efects are restricted to food categories and do not involve non-food categories. Moreover, several values of cross-purchase efects for the same two categories are clearly diferent in two segments (e.g., yogurt on milk: 0.0094 in segment 1 and 0.0030 in segment 4; carbonated beveragse on salty snacks: 0.0084 in segment 5 and 0.0122 in segment 6; toilet tissue on paper towels: 0.0032 in segment 1 and 0.0048 in segment 5).

Obtained clusters of categories and category pairs

As interpretation aid for the RC-SVML model we cluster an undirected graph whose nodes represent categories and category pairs in accordance with ["Clustering categories and](#page-7-0) [category pairs](#page-7-0)" section. Maximizing modularity yields four clusters, which are described in Table [15](#page-11-1). Four categories (beer & ale, cigarettes, diapers, photographic supplies) are isolated and consequently do not belong to any cluster.

Cluster 1 contains non-food categories (deodorant, blades, razors). It also contains seven pairs and three pairs in which the categories blades and deodorants participate, respectively. Only food categories (salty snacks, spaghetti sauce, margarine & butter, mustard & ketchup, mayonnaise, frankfurters & hotdog, carbonated beverages) are assigned to cluster 2. Its category pairs involve food categories only. Cluster 3 consists of non-food categories (paper towels, toilet tissue, shampoo, tooth paste, laundry detergent, household cleaners, facial tissue, tooth brush) except for coffee. Cluster 4 contains food categories only (cold cereal, yoghurt, peanut butter, milk, soup, frozen pizza, frozen dinners, sugar substitutes). In a comparable manner its category pairs involve food categories. Overall, these descriptions show clear diferences between clusters.

Categories with a high number of links to other categories and category pairs can be rated as central for a cluster. This centrality measure is known as degree of a node and frequently used to characterize graphs (Diestel [2005\)](#page-14-35). Cluster-specifc central categories are:

Table 16 Diferences of feature efects between the RC-SMVL and RC-MVL models

Featured cat- egory	Affected cat- egory	RC-SMVL	RC-MVL	Difference
	Negative differences \le - 0.0010			
coldcer	coldcer	0.0158	0.0198	$= 0.0040$
spagsauc	spagsauc	0.0138	0.0172	-0.0034
beer	beer	0.0014	0.0038	-0.0024
saltsnck	saltsnck	0.0168	0.0188	-0.0020
soup	soup	0.0100	0.0116	-0.0016
fzdin	coldcer	0.0000	0.0014	-0.0014
soup	coldcer	0.0000	0.0014	-0.0014
paptowl	paptowl	0.0032	0.0046	-0.0014
peanbutr	peanbutr	0.0038	0.0052	-0.0014
coffee	coldcer	0.0000	0.0012	-0.0012
margbutr	coldcer	0.0000	0.0012	-0.0012
factiss	factiss	0.0040	0.0052	-0.0012
carbbev	saltsnck	0.0020	0.0032	-0.0012
fzpizza	saltsnck	0.0000	0.0012	-0.0012
milk	coldcer	0.0000	0.0010	-0.0010
fzpizza	fzpizza	0.0098	0.0108	-0.0010
spagsauc	margbutr	0.0000	0.0010	$= 0.0010$
laundet	paptowl	0.0000	0.0010	-0.0010
coffee	spagsauc	0.0000	0.0001	-0.0010
coldcer	spagsauc	0.0006	0.0016	-0.0010
spagsauc	yogurt	0.0000	0.0010	$= 0.0010$
Positive differences ≥ 0.0010				
toitisu	toitisu	0.0084	0.0056	0.0028
diapers	diapers	0.0020	0.0006	0.0014
margbutr	margbutr	0.0096	0.0082	0.0014
mayo	mayo	0.0060	0.0046	0.0014
milk	milk	0.0170	0.0156	0.0014
fzpizza	laundet	0.0000	-0.0010	0.0010
toitisu	laundet	0.0010	0.0000	0.0010
yogurt	yogurt	0.0112	0.0102	0.0010

Only contains feature efects with diferences at least 0.0010 in absolute size

- razors (22) for cluster 1.
- mustard & ketchup (18) and hotdog & frankfurters (13) for cluster 2.
- toilet tissue (28), paper towels (19) and laundry detergent (14) for cluster 3.
- cold cereal (6) and soup (25) for cluster 4.

Fig. [1](#page-5-3) contains directed graphs for each of these four clusters. Directed links indicate that a category or category pair afects another category. One can also see from these graphs which categories are central for a cluster.

Managerial implications

We indicate what the RC-SMVL model implies with respect to cross selling. Cross-selling can be be supported by recommending categories not purchased, e.g. by printing at checkout or as part of a mobile phone message. Such recommendations can be based on high positive interactions (see Tables [7,](#page-7-1) [8](#page-7-2) and [9](#page-8-1)). For example, the category shampoo (frozen dinner) can be recommended if the basket of a customer contains tooth paste and deodorants (frozen pizza and soup).

Segment-specifc recommendations require that a household be allocated to the segment with the highest log pseudolikelihood across observed purchase categories. Recommendations can rely on higher positive cross-purchase efects (see Tables [12,](#page-9-2) [13](#page-10-1) and [14](#page-10-2)). Category yoghurt (soup) can be recommended to a household of segment 3 (7) purchasing cold cereal and soup (cold cereal and spaghetti sauce). Across all segments the category salty snacks can be recommended to a households purchasing carbonated beverages and cold cereal.

Management may enhance dross-selling also by appropriate positioning of categories in aisles and shelves of a store. Categories exert more efects on other categories belonging to the same cluster (see "[Obtained clusters of categories and](#page-11-0) [category pairs"](#page-11-0) section). Categories belonging to the same cluster are placed near to each other (e.g., carbonated beverages and salty snacks near to each other and far away from categories such as cold cereal and milk). Central categories can be positioned in the middle of the other categories belonging to the same cluster (e.g., mustard & ketchup and hotdog & frankfurters for cluster 2, cold cereal and soup for cluster 4). Isolated categories on the other hand at g (e.g., beer & ale, photographic supplies) can be positioned at greater distances to products belonging to a cluster.

Next, we assess whether managerial implications with respect to category-specifc features vary between the RC-SMVL and RC-MVL models. To this end we compute differences of their respective feature efects. Feature efects are measured by the diference of purchase probabilities of category *j* between high and low values of features for category *j*. For $j' = j$ we obtain an own effect, otherwise a cross efect. High (low) values of features for category *j* result from multiplying their average value by a multiplicative factor greater (less) than zero. We set this factor to 1.1 (0.9) and keep values of loyalties and features of other categories $j' \neq j$ at their average values.

Please note that the estimated coefficients presented in expressions (4) (4) , (7) (7) and (12) (12) (12) refer to conditional probabilities and do not directly refect efects on unconditional purchase probabilities. To determine unconditional purchase probabilities, we generate simulated purchases by iterated Gibbs-sampling from the appropriate conditional distribution (Besag [2004](#page-14-30)). In case of the RC-SMVL and RC-MVL **Table 17** Feature efects of the RC-SMVL model

Only contains feature effects at least 0.0020 in absolute size

models, we generate simulated purchases for each of 500 sampled category constants and coefficients. We estimate the unconditional purchase probability of a category by its marginal relative frequency across the simulated purchases.

Table [16](#page-12-1) shows that only five of the total 930 (= 31×30) feature efects difer between the RC-SMVL and RC-MVL models by at least 0.0020 in absolute size. All these five are own effects (cold cereal, spaghetti sauce, beer $\&$ ale, salty snacks, toilet tissue). Especially for zero feature effects that the RC-SVML model implies in contrast to the RC-MVL model, diferences are not greater than 0.0010 in absolute size, many of these are much smaller. We therefore conclude that managerial implications with respect to feature efects are as a rule very similar for the two models.

Feature effects implied by the RC-SMVL of at least 0.0020 in absolute size are given in Table [17](#page-13-1). These effects are all positive, i.e., higher features increase the uncondi-tional purchase probability of the affected category. Table [17](#page-13-1) contains own efects with the exception of one cross efect (features for salty snacks afect purchases of carbonated beverages).

Conclusion

We introduce a sparse multivariate logit (SVML) model to analyze market basket data. In contrast to the conventional multivariate logit (MVL) model the SVML model that does not include all two-way interactions between product categories. A combined forward and backward selection procedure based on a cross-validated performance measure excludes most two-way interactions. Because of its lower complexity the SVML clearly outperforms the MVL model in terms of the Bayesian information criterion (BIC). Random coefficient versions of these models (RC-MVL and RC-SVML) further improve performance demonstrating that latent heterogeneity of households is important. Once again, the sparse variant RC-SVML beats the non-sparse variant RC-MVL in terms of BIC.

For our data set only about 26 % of all possible two-way interactions remain in the RC-SVML. This result facilitates interpretation of the RC-SVML in comparison to the RC-MVL model. As further interpretation aid we determine four clusters of categories and category pairs by maximizing modularity using the interaction coefficients detected by the RC-SVML model. As a rule, these four clusters contain either food or non-food categories. Four categories are isolated, i.e., they are not part of an interaction effect.

We show what the estimated RC-SVML model implies for cross-selling based on product recommendations and store layout. Moreover, we measure efects of increasing features (advertising in local newspapers and fyers) on the purchase probability of categories. Most feature efects turn out to be equal for the two models. Only 0.5 % of all possible efects difer by at least 0.002 in absolute size between the SVML and the MVL models. To sum up, the sparse model attains a better statistical performance if model complexity is taking into account and offer better interpretability. In addition to these advantages, the sparse model leads to managerial implications with respect to feature efects that are as a rule close to those implied by its non-sparse counterpart.

The data that we use in this paper originate from a food retailing context. The presented approach could be readily applied to purchases of non-food product categories or browsing behavior across pages of a website or across multiple websites. Moreover, future research efforts might extend our approach in several ways. One possibility consists in analyzing purchases at a more detailed level (e.g., the brand level). Moreover, binary purchase incidences could be replaced or supplemented by response variables like purchase amount and purchase quantity.

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Data availability The dataset used in the current study is not publicly available as it contains proprietary information that the authors acquired through a license. Information on how to obtain it and reproduce the analysis is available from the corresponding author on request.

Declarations

Conflict of interest The author states that there is no confict of interest.

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