Learning Consumer Preferences from Bundle Sales Data

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Abstract. Product bundling is a common selling mechanism used in online retailing. To set profitable bundle prices, the seller needs to learn consumer preferences from the transaction data. When customers purchase bundles or multiple products, classical methods such as discrete choice models cannot be used to estimate customers’ valuations. In this paper, we propose an approach to learn the distribution of consumers’ valuations toward the products using bundle sales data. The approach reduces it to an estimation problem where the samples are censored by polyhedral regions. Using the EM algorithm and Monte Carlo simulation, our approach can recover the distribution of consumers’ valuations. The framework allows for unobserved no-purchases and clustered market segments. We provide theoretical results on the identifiability of the probability model and the convergence of the EM algorithm. The performance of the approach is also demonstrated numerically.

Keywords: EM algorithm · bundle · censored demand · clustering

1 Introduction

Bundles are pervasive in online retailing, fast-food restaurants, and the video game industry. Companies bundle products and services together at a bargain price to boost the demand of customers. Many firms in various markets—from combo deals in McDonald’s, discounts for home and auto policies combined for insurance companies, to deals for flights as a package of a price, the number of baggage and meals for airlines—use bundling as one of their main promotion strategies. Due to the popularity of bundles, how to set profitable bundle pricing strategies has been a focus of the literature since Stigler (1963). A number of simple bundle pricing strategies have shown promising theoretical and empirical performance, such as grand bundles (bundling all products together at a discount) and bundle size pricing (pricing the bundle based on its size only). See Chu, Leslie, and Sorensen (2011) for a comprehensive empirical comparison.

A prerequisite for almost all successful bundle pricing schemes is the accurate estimation of consumers’ reservation prices or valuations. That is, how consumers react to a price menu of products and bundles in the form of aggregate market demand. A typical source of data to learn such information is the past transaction data that the firm has collected. However, compared to the number of studies on how to set prices for bundles assuming known market demand or valuation distributions, there is scant literature on how to learn the valuations from the transaction data of bundle sales. This is a stark contrast to the industry practice: according to Fisher et al. (2020), companies make more than 90% of the effort estimating demand and 10% setting optimal prices.

This study focuses on learning consumer valuations from the transaction data of bundle sales, which allows the firm to set profitable bundle pricing strategies. In a sense, our study can be viewed as a preprocessing step for developing bundle pricing strategies. The firm observes the behavior of past customers: the products and bundles that are offered at the time, the charged prices, and the final purchase decisions. Based on the information, the firm attempts to learn the valuations of the customers in the data to forecast the shopping behavior of future customers.

The challenges of this learning problem arise from missing values, censored data, and bundle promotion. We next summarize each of these challenges and the reason for the insufficiency of existing approaches. First, customers’ value for products is missing values in sales data. While customers’ purchase decisions are observed in sales data, the realized valuations are not. That is, the firm only observes that a past customer is willing to pay $5 for a t-shirt, but it doesn’t know if the customer values the t-shirt at $7 or $10. Second, demand censoring, which refers to the common issue that customers who don’t make any purchases are not observed in the sales data, also plagues the studied estimation problem. The first two challenges are common
for estimation problems based on sales data. The method used to uncensored data for discrete choice models without bundles cannot be directly applied. For transaction data without bundles, discrete choice models such as the multinomial logit (MNL) model tackle the challenge by linking the purchase probabilities to the parameters without observing the valuations directly. In the presence of bundles, discrete choice models can be applied if one views a bundle as an independent product. But such an arrangement neglects the connection between bundles and the component products. This is another unique problem when the transaction data include bundle sales. Therefore, the third challenge of products commonly bundled together hurdles the use of existing methods. When products are bundled together, the valuations for these products are entangled. When a customer purchases the bundle, it is unclear which product the customer has valued higher. Therefore, it is challenging for the firm to learn products’ valuations among customers separately.

In this paper, we construct a simple model for consumer valuations and provide an algorithm to estimate the parameters from the data. In particular, we assume the valuations customers have toward the products have a multivariate Gaussian distribution. For a bundle, the valuation is the sum of the valuations of the component products. Such an additive utility model is commonly used in the bundle pricing literature. We formulate the problem as a maximum likelihood estimation with incomplete data where customers' valuation samples are not observed. We then design an algorithm combining the expectation-maximization (EM) algorithm and Monte Carlo simulation to estimate the mean and covariance matrix of the Gaussian distribution. The contribution of the paper is threefold.

– We show the equivalence between the problem and another estimation problem that is of independent interest. We find the transaction data can be converted to censored samples of customer valuations. More precisely, the transaction data does not reveal the exact location of the valuations of each customer, but record a polyhedral region with linear boundaries in which the sample falls in. A special case of this problem, interval-censored data, is commonly seen in survival analysis (Lindsey and Ryan 1998). Our formulation generalizes the interval to polyhedra in high dimensions.

– The framework and algorithm we propose are flexible enough to accommodate many realistic considerations. We extend the framework to allow for Gaussian mixture models (GMM). Therefore, customers may have clustered valuations due to market segmentation and any distribution can be approximated. Our framework can tackle censored demand. Computationally, we demonstrate the algorithm on a synthetic dataset with 6 products, 42 bundles, and 4000 transactions. This is because Monte Carlo simulation allows us to provide close-form updates in the M-step. No known algorithms can handle the estimation problem for bundle sales of this scale.

– We answer two theoretical questions: when is the model identifiable, and whether the proposed algorithm converges to the true parameters. Both questions have not been answered before for the estimation problem with bundle sales. For the first question, we identify a simple pricing policy used by many firms that leads to identifiable transaction data. For the second question, we leverage the recent advances (Balakrishnan, Wainwright, and Yu 2017) and show that the algorithm is guaranteed to converge linearly to a neighborhood of the true parameters (global maximum of the likelihood function) under a number of technical conditions. The convergence to the global maximum is only established recently and we are the first to show such a result for the problem we study.

2 Literature Review

Bundle pricing mechanisms have been studied extensively in the literature, including their theoretical and computational properties. We list a number of representative papers below. Bakos and Brynjolfsson (1999), Abdallah, Asadpour, and Reed (2021) analyze the asymptotic performance of pure bundling and bundle size pricing. Chu, Leslie, and Sorensen (2011) conduct a comprehensive numerical experiment to compare the performance of four commonly studied bundle pricing mechanisms. Hanson and Martin (1990), Wu, Hitt, Chen, and Anandalingam (2008), Jiang, Shang, Kemerer, and Liu (2011), Li, Sun, and Teo (2020) provide mixed-integer programming or convex optimization formulations to compute the optimal bundle pricing policies. Hart and Nisan (2017), Babaioff, Immorlica, Lucier, and Weinberg (2020) derive theoretical performance bounds for simple mechanisms. A few recent studies (Ma and Simchi-Levi 2021, Sun, Li, and Teo 2021, Chen, Li, Li, and Wang 2022) propose new implementable pricing mechanisms and analyze their properties. These papers usually rely on one crucial assumption: the distribution of consumers’ valuations is
known or a number of realized samples are given. In practice, however, such information needs to be learned from the sales data. Our work provides a framework to achieve this goal and further justifies the practical feasibility of the pricing mechanisms studied in these papers. As pointed out by Fisher, Olivares, and Staats (2020), the estimation of demand (customers’ valuations) is 90% of the work in practice.

Our work is related to the stream of literature that focuses on the estimation of discrete choice models, especially the well-known multinomial logit (MNL) model, from transaction data. Kök et al. (2008) provide a comprehensive literature review of the earlier studies on such models in revenue management. Building on Talluri and Van Ryzin (2004), Vulcano et al. (2012) combine the MNL model with a non-homogeneous Poisson arrival process over multiple periods and use the EM algorithm to estimate model parameters as well as the number of no-purchases. Newman et al. (2014) incorporate price and product features into their estimation approach. Abdallah and Vulcano (2021) study the identifiability of this type of model and propose a computational approach to optimize the likelihood function. Subramanian and Harsha (2021) use a mixed-integer program to estimate the parameters under the loss-minimization objective function. The estimation of other types of discrete choice models is also studied, including the rank-based choice model (Farias, Jagabathula, and Shah 2013, Van Ryzin and Vulcano 2015) and the Markov chain choice model (Şimşek and Topaloglu 2018). The major contribution of this paper to the literature is that we consider customers may purchase bundles that a firm offer at a discount. Such a setting doesn’t fit into the classic discrete choice models, and this estimation problem has not been studied in the literature.

This study proposes a framework to estimate the customers’ valuations from transaction data for multiple products when the firm may offer a price menu for products and bundles. There are three closely related papers (Jedidi, Jagpal, and Manchanda 2003, Letham, Sun, and Sheopuri 2014, Ma and Simchi-Levi 2020) in this domain. Jedidi et al. (2003) study a similar problem and propose a hierarchical Bayesian approach to infer the parameters of a multivariate Gaussian distribution that is used to model the valuations for the products. However, they propose to use off-the-shelf Bayesian computational tools that seem to suffer from computational issues when the number of products is moderate or large, according to our experiments. Indeed, their numerical experiments are conducted for only two products and one bundle. Instead, we provide an analytical framework to study this problem and use the EM algorithm and Monte Carlo simulation to estimate the model parameters. We show that the problem can be translated to an estimation problem when the samples are “censored by regions”, i.e., the exact locations of the samples are not observed but a polyhedral region in which each sample falls is given. In another related paper, Letham et al. (2014) approximate the polyhedral region with rectangular regions, which allows them to simplify the likelihood function. In contrast, we use the EM algorithm to solve the original estimation problem without approximations. Ma and Simchi-Levi (2020) consider a slightly different setting: the bundle discount is only offered when a customer purchases all products. They do not assume a parametric form for the valuation distribution and focus on a few quantities of interest, in order to reconstruct linear demand curves of each product. They show their estimators are consistent. Our setting assumes the Gaussian distribution and allows for an arbitrary price menu. In addition to the different setups and methodologies, we extend our approach to the censored demand (unobserved no-purchases). This is not considered in Jedidi et al. (2003), Letham et al. (2014), Ma and Simchi-Levi (2020).

The methodology used in this paper, the EM algorithm combined with Monte Carlo simulation, has been used in previous studies, including Natarajan et al. (2000), Lee and Scott (2012). In particular, Monte Carlo simulation is used to approximate the E-step, when the expectation doesn’t have a closed form. Because our study is focused on a specific practical problem, we provide the concrete steps of the EM algorithm and the Monte Carlo simulation. Moreover, the theoretical properties are derived for the bundle application. In general, the EM algorithm is only guaranteed to converge to the local maximum of the sample likelihood function. Balakrishnan et al. (2017) provide conditions and statistical guarantees for the EM algorithm to converge to the global maximum of the likelihood function i.e., the true parameters, when initialized in a neighborhood. We prove that the conditions proposed by Balakrishnan et al. (2017) hold for our problem.

3 The Data Model and Estimation

In this section, we first introduce the format of the dataset recording the bundle transactions. Suppose there are $I$ products and we use $[I] ≜ \{1, \ldots, I\}$ to denote the product space. There are $J$ candidate bundles offered on the menu and we use $j \in \{0, 1\}^I$ to denote a bundle. That is, product $i \in [I]$ is included in
bundle $j$ if and only if $j_i = 1$. Note that not all the bundles are offered to each customer and a bundle may include only one product. With a little abuse of notation, we also use $j$ as the bundle index in the menu $[J] \triangleq \{1, \ldots, J\}$ and $i \in j$ when bundle $j$ includes product $i$.

The dataset records the purchase of $N$ customers: customer $n \in [N] \triangleq \{1, \ldots, N\}$ chooses bundle $c_n \in [J] \cup \{0\}$, where the choice 0 stands for no purchases. The case of censored demand is investigated in Section 4.1. Moreover, the price of bundle $j$ faced by customer $n$ is denoted by $p_n^j$, which is also recorded in the dataset. Therefore, the dataset consists of the tuples $(p_n^1, \ldots, p_n^J, c_n)^{N}_{n=1}$. Note that we do not require the offering of all the bundles in the menu to all the customers. When a customer is only offered a subset of the available bundles, we can artificially set the prices of the bundles that are not offered to infinity.

To be able to utilize the dataset and estimate customer preferences, we specify a utility model. Suppose customer $t$ is endowed with a vector of valuations, $v_n = (v_1, \ldots, v_J)$, for the products. Under additive utility, the valuation for bundle $j$ is $\sum_{i \in j} v_i$. Note that additive utility is a standard assumption in the literature, although other types of valuation functions have been proposed and studied recently. For additive utility, the complementary or substitutability of products can be captured by the correlation of the valuations.

Under this utility model, the choice $c_n = j \neq 0$ corresponds to the following region of the valuation vector $v$, given by the incentive-compatible constraints:

$$c_n = j \iff \left\{ \sum_{i \in j} v_i - p_n^j \geq \max_{j' \in J \setminus j} \sum_{i \in j'} v_i - p_n^{j'}, \sum_{i \in J} v_i - p_n^j \geq 0 \right\}. \quad (1)$$

Similarly, we have

$$c_n = 0 \iff \left\{ \max_{j' \in J \setminus j} \sum_{i \in j'} v_i - p_n^{j'} \leq 0 \right\}. \quad (2)$$

Suppose the valuation $v$ of each customer is independently drawn from an $J$-dimensional multivariate normal distribution:

$$v \sim \mathcal{N}(\mu, \Sigma). \quad (3)$$

Note that we focus on the somewhat restrictive normal distribution for the purpose of exposition. In Section 4.2, we relax it to a Gaussian mixture model, which is flexible enough to approximate any probability distributions (for example, see (Goodfellow et al. 2016, p.65)).

With the presented data model, now we can state the goal of the firm. Given the dataset $\{(p_n^1, \ldots, p_n^J, c_n)\}^{N}_{n=1}$, the firm wants to estimate the distribution of the customer valuations, in particular $\mu$ and $\Sigma$, with the knowledge that the incentive-compatible constraints (1) and (2) relate the valuations to the observations in the dataset. Note that precisely because of this indirect relationship, this problem is not standard in the statistics literature. For example, if $v_n$ were observed, then the estimation of $\mu$ and $\Sigma$ would be trivial using the empirical average and covariance matrix of $\{v_n\}^{N}_{n=1}$. Next we explain how the problem can be viewed as an estimation problem with missing data and present an algorithm for the problem.

### 3.1 An Estimation Problem with Missing Data

The key observation to simplify the estimation problem is that given $(p_n^1, \ldots, p_n^J, c_n)$, the incentive-compatible constraints (1) and (2) specify a polyhedron in which the valuation vector $v_n$ falls in. More precisely, define

$$R_n^j \triangleq \left\{ v : \sum_{i \in j} v_i - p_n^j \geq \max_{j' \in J \setminus j} \sum_{i \in j'} v_i - p_n^{j'}, \sum_{i \in J} v_i - p_n^j \geq 0 \right\}, \quad j \neq 0,$$

$$R_n^0 \triangleq \left\{ v : \max_{j' \in J \setminus j} \sum_{i \in j'} v_i - p_n^{j'} \leq 0 \right\}. \quad (4)$$

which we refer to as IC polyhedra. The observation $c_n = j$ is equivalent to $v_n \in R_n^j$. As a result, for customer $n$, the valuation space $\mathbb{R}^J$ can be partitioned into the $J + 1$ regions: $\mathbb{R}^J = \bigcup_{j=1}^{J+1} R_n^j \cup R_n^0$. The observation $(p_n^1, \ldots, p_n^J, c_n)$ characterizes the partition as well as the IC polyhedron in which $v_n$ falls. Therefore, instead
we are interested in estimating \((\mu, \Sigma)\), the distribution of the valuations for the products among consumers. By convention, we use \(\theta \triangleq (\mu, \Sigma)\) to denote the parameters.

**Parameters:** we are interested in estimating \((\mu, \Sigma)\), the distribution of the valuations for the products among consumers. By convention, we use \(\theta \triangleq (\mu, \Sigma)\) to denote the parameters.

**Observed data:** the firm observes the polyhedra \(\{R_{v_n}^c\}_{n=1}^N\) given the data \(\{(p_{v_n}^1, \ldots, p_{v_n}^d, c_n)\}_{n=1}^N\) in (4). We use \(X \triangleq \{R_{v_n}^c\}_{n=1}^N\) for the observed data. Note that by converting the data to polyhedra, we do not lose any information regarding the possible valuations \(\{v_n\}_{n=1}^N\).

**Missing data:** we treat valuations \(v_n, n = 1, \ldots, N\), as the missing data. They are related to the observed data by the simple fact that \(v_n \in R_{v_n}^c\). We use \(Z \triangleq \{v_n\}_{n=1}^N\) for the missing data.

There are two common approaches to missing data: imputation and maximum likelihood estimator (MLE). Since our estimation problem is model-based, we adopt the latter. In particular, the likelihood function based on the observed data is:

\[
L(\theta; X) = \int p(X, Z|\theta) dZ = \prod_{n=1}^N \int_{R_{v_n}^c} f(v|\mu, \Sigma) dv,
\]

where

\[
f(v|\mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp \left(-\frac{1}{2}(v - \mu)^T \Sigma^{-1}(v - \mu)\right)
\]

is the probability density function (PDF) of the multivariate normal distribution (3).

To maximize the likelihood function over \(\theta\), a standard technique is to apply logarithm to the likelihood function and maximize the log-likelihood function instead. However, because of the integration, the optimization is theoretically intractable and computationally challenging. As a popular alternative, the EM algorithm iteratively maximizes the likelihood function by focusing on the complete-data likelihood. Next we elaborate on the implementation of the EM algorithm in this problem.

### 3.2 The EM Algorithm

Instead of focusing on the (log-)likelihood function of the observed data with missing values, the EM algorithm focuses on the complete-data log-likelihood function, i.e.,

\[
l(\theta; X, Z) = \sum_{n=1}^N \log f(v_n|\mu, \Sigma).
\]

Note that as an objective function, \(l(\theta; X, Z)\) is a lot easier to handle than \(l(\theta; X)\); because of the form of \(f\) (belonging to the exponential family), the complete-data log-likelihood is a quadratic function, which is easy to optimize. However, \(Z\) is not observed from the data.

The EM algorithm circumvents the issue by estimating \(\theta^{(t)}\) iteratively. In each iteration, suppose \(\theta^{(t)} = (\mu^{(t)}, \Sigma^{(t)})\) is given. We first evaluate the expected complete-data log-likelihood over \(Z\), i.e.,

\[
Q(\theta^{(t)}) \triangleq \mathbb{E} \left[l(\theta; X, Z) \bigg| X, \mu^{(t)}, \Sigma^{(t)}\right] = \sum_{n=1}^N \int_{R_{v_n}^c} f(v|\mu^{(t)}, \Sigma^{(t)}) dv \log f(v|\mu, \Sigma) dv.
\]

This is the so-called E-step and the expectation is taken with respect to the missing data \(Z\). Given \((X, \mu^{(t)}, \Sigma^{(t)})\), the missing variable \(v_n\) has a conditional Gaussian distribution inside the polyhedron \(R_{v_n}^c\) with the given mean and covariance. Its PDF is thus \(f(v|\mu^{(t)}, \Sigma^{(t)}) / \int_{R_{v_n}^c} f(x|\mu^{(t)}, \Sigma^{(t)}) dx\) for \(v \in R_{v_n}^c\), which is the first term in the integral. The second term \(\log f(v|\mu, \Sigma)\) is the log-likelihood function \(l(\theta; X, Z)\) and is integrated with the conditional PDF for its expected value.
To find a new estimator for $\theta$ in the $t$-th iteration, the $M$-step in the EM algorithm maximizes $Q(\theta | \theta^{(t)})$ and let $\theta^{(t+1)} = \arg\max_{\theta} Q(\theta | \theta^{(t)})$. However, the major difficulty is to deal with the integral and the denominator which don’t have closed forms. To deal with this challenge, we use Monte Carlo simulation. More precisely, for all $n = 1, \ldots, N$, we simulate $L$ samples according to the same distribution as $v | R_n^c, \mu(t), \Sigma(t)$. This is the conditional multivariate normal distribution inside $R_n^c$. The standard acceptance-rejection method can be used and we provide the details in Algorithm 1.

Algorithm 1 Acceptance-rejection method

```
1: Input: $R_n^c$, $\mu(t)$, $\Sigma(t)$, $L$
2: $l \leftarrow 1$
3: while $l \leq L$ do
4:   Repeat $x \sim \mathcal{N}(\mu(t), \Sigma(t))$ until $x \in R_n^c$
5:   $x^{(l)} \leftarrow x$
6:   $l \leftarrow l + 1$
7: end while
8: return $\{x^{(1)}, \ldots, x^{(L)}\}$
```

Once the Monte Carlo samples $\{x^{(l)}_n\}$ for $n = 1, \ldots, N$ and $l = 1, \ldots, L$ have been generated, we may replace $Q(\theta | \theta^{(t)})$ in (6) by

$$
\hat{Q}(\theta | \theta^{(t)}) = \frac{1}{L} \sum_{n=1}^{N} \sum_{l=1}^{L} \log f(x^{(l)}_n | \mu, \Sigma)
= C + \frac{1}{L} \sum_{n=1}^{N} \sum_{l=1}^{L} \left( -\frac{1}{2} (x^{(l)}_n - \mu)^\top \Sigma^{-1} (x^{(l)}_n - \mu) - \frac{1}{2} \log \det \Sigma \right),
$$

where $C$ is constant with respect to $\mu$ and $\Sigma$. Note that this is the standard MLE for multivariate normal distribution with $NL$ samples. Therefore, we have

$$
\mu^{(t+1)} = \frac{1}{NL} \sum_{n=1}^{N} \sum_{l=1}^{L} x^{(l)}_n,
\Sigma^{(t+1)} = \frac{1}{NL} \sum_{n=1}^{N} \sum_{l=1}^{L} (x^{(l)}_n - \mu^{(t+1)}) (x^{(l)}_n - \mu^{(t+1)})^\top.
$$

This completes the $t$-th iteration of the EM algorithm.

The EM algorithm is terminated when the estimation $\theta^{(t)}$ has converged. In practice, we may impose a small tolerance level $\epsilon > 0$ and terminate the algorithm once $\|\theta^{(t+1)} - \theta^{(t)}\| \leq \epsilon$ for a chosen norm $\| \cdot \|$. We summarize the steps in Algorithm 2.

**Sampling efficiency of Monte Carlo simulation.** In practice, the major computational complexity of Algorithm 2 is caused by the Monte Carlo simulation. In particular, when the region $R_n^c$ is small or distant from $\mu(t)$, Algorithm 1 may be inefficient as it requires a large number of samples in Step 4 to draw one accepted in $R_n^c$. We provide three remedies to improve the sampling efficiency.

First, in each iteration of Algorithm 2 (Step 4), we can generate a large number of samples from $\mathcal{N}(\mu(t), \Sigma(t))$ and store them. When running Algorithm 1 for each $R_n^c$, the algorithm can use the same set of samples for acceptance/rejection. This saves the computation time to generate a large number of samples for each $n = 1, \ldots, N$.

Second, we may not require the same number of samples $L$ in all regions $R_n^c$. For example, we may simulate $L_n$ Monte Carlo samples for region $R_n^c$ so that $L_n$ could be smaller for low-probability $R_n^c$. As long as we use $\sum_{t=1}^{L_n} \log f(x^{(l)}_n | \mu, \Sigma)/L_n$ in $\hat{Q}(\theta | \theta^{(t)})$, it is still unbiased. However, one needs to caution that the Monte Carlo error is bottlenecked by the smallest $L_n$. 


choosing \( \mu \) estimate \( Q \) challenging as Step 4 is repeated many times before acceptance. Instead, we can consider a different normal particular, consider (6) and some

Algorithm 2 The EM algorithm

1: Input: \( \{ p^i_n, \ldots, p^j_n, c_n \}_{n=1}^N \), \( \epsilon \), \( L \), \( \mu^{(0)} \), \( \Sigma^{(0)} \)
2: Calculate \( \{ R^{(c)}_{n} \}_{n=1}^N \) from the data according to (4)
3: \( error \leftarrow 100 \), \( t \leftarrow 0 \)
4: while \( error > \epsilon \) do
5: \( \text{Run Algorithm 1 for } \{ R^{(c)}_{n} \}_{n=1}^N \)
6: Update
   \[
   \mu^{(t+1)} \leftarrow \frac{1}{NL} \sum_{n=1}^N \sum_{l=1}^L x_n^{(l)}
   \]
   \[
   \Sigma^{(t+1)} \leftarrow \frac{1}{NL} \sum_{n=1}^N \sum_{l=1}^L \left( x_n^{(l)} - \mu^{(t+1)} \right) \left( x_n^{(l)} - \mu^{(t+1)} \right)^T
   \]
7: \( error \leftarrow \| \mu^{(t+1)} - \mu^{(t)} \|_1 + \| \Sigma^{(t+1)} - \Sigma^{(t)} \|_1 \), \( t \leftarrow t + 1 \)
8: end while
9: return \( \mu^{(t)} \), \( \Sigma^{(t)} \)

Third, for low-probability \( R^{(c)}_{n} \), we may use importance sampling to increase the sampling efficiency. In particular, consider (6) and some \( n \) that \( f(v|\mu^{(t)}, \Sigma^{(t)}) \approx 0 \) for \( v \in R^{(c)}_{n} \). In this case, it is computationally challenging as Step 4 is repeated many times before acceptance. Instead, we can consider a different normal distribution \( N(\mu', \Sigma') \) such that \( v \in R^{(c)}_{n} \) with high probability. This can be achieved, for example, by choosing \( \mu' \) close to the center of \( R^{(c)}_{n} \) when \( R^{(c)}_{n} \) is bounded. As a result, we have

\[
\begin{align*}
\int_{v \in R^{(c)}_{n}} f(v|\mu^{(t)}, \Sigma^{(t)}) \log f(v|\mu, \Sigma) \, dv &= \int_{v \in R^{(c)}_{n}} f(v|\mu', \Sigma') \int_{R^{(c)}_{n}} f(x|\mu', \Sigma') \, dx \log f(v|\mu, \Sigma) \, dv \\
&= \frac{1}{\int_{R^{(c)}_{n}} f(x|\mu', \Sigma') \, dx} \sum_{l=1}^L f(x_n^{(l)}|\mu', \Sigma') \sum_{l=1}^L f(x_n^{(l)}|\mu, \Sigma) \log f(x_n^{(l)}|\mu, \Sigma),
\end{align*}
\]

where the equality follows from approximating the denominator outside the sum:

\[
\begin{align*}
\int_{R^{(c)}_{n}} f(x|\mu^{(t)}, \Sigma^{(t)}) \, dx &= \int_{R^{(c)}_{n}} \frac{f(x|\mu^{(t)}, \Sigma^{(t)})}{f(x|\mu', \Sigma')} \frac{f(x|\mu', \Sigma')} {f(x_n^{(l)}|\mu, \Sigma')} \, dx = \frac{1}{L} \sum_{l=1}^L f(x_n^{(l)}|\mu^{(t)}, \Sigma^{(t)}).
\end{align*}
\]

We define \( w_{ni} \triangleq \frac{f(x_n^{(l)}|\mu^{(t)}, \Sigma^{(t)})}{f(x_n^{(l)}|\mu', \Sigma')} / \sum_{l=1}^L f(x_n^{(l)}|\mu^{(t)}, \Sigma^{(t)}) \). Using the Monte Carlo samples, and (8), the approximate Q function (6) can be cast in the following form

\[
\hat{Q} (\theta|\theta^{(t)}) = \sum_{n=1}^N \sum_{l=1}^L w_{ni} \log f(x_n^{(l)}|\mu, \Sigma).
\]
The $M$-step thus leads to the following update

$$
\mu^{(t+1)} = \frac{\sum_{n=1}^{N} \sum_{l=1}^{L} w_{nl} x_{n}^{(l)}}{\sum_{n=1}^{N} \sum_{l=1}^{L} w_{nl}},
$$

$$
\Sigma^{(t+1)} = \frac{\sum_{n=1}^{N} \sum_{l=1}^{L} w_{nl} \left( x_{n}^{(l)} - \mu^{(t+1)} \right) \left( x_{n}^{(l)} - \mu^{(t+1)} \right)^{\top}}{\sum_{n=1}^{N} \sum_{l=1}^{L} w_{nl}}.
$$

Therefore, using importance sampling results in a similar procedure to Algorithm 2 but reduces the computation in Algorithm 1.

## 4 Model Extensions

In this section, we consider two extensions of the base model in Section 3.

### 4.1 Censored Demand

In practice, the transactions observed by the firm are typically censored: the firm only records the transactions in which customers purchase at least one item and the customers who have not purchased anything are censored. Next we tackle this problem using our framework.

For ease of exposition, in this subsection, we consider that the firm propose only one price menu $p = (p^1, \ldots, p^J)$ seen by all customers. Therefore, we assume that the firm observes $(p^3, \ldots, p^J, c_n)$ for customer $n$, where the choice $c_n > 0$ for $n = 1, \ldots, N$. This data can be converted to the IC polyhedron defined in (4), \{R^0, R^1, \ldots, R^J\}. Note that they are constant for all customers because of the fixed price menu. Similarly we treat $v_n, n = 1, \ldots, N$, the valuation of customer $n$, as the missing data.

Because of the demand censoring, the total number of customers that have visited the store, $N' \geq N$, is also unobserved, as well as the valuations of the censored customers $v_n, n = N + 1, \ldots, N'$. Therefore, the missing data is $Z \triangleq \{N', v_1, \ldots, v_{N'}\}$. It is known that $v_n \in R^0$ for the censored customers $n = N+1, \ldots, N'$. Moreover, we record the total number of customers that buy bundle $j$ as $N_j$, where $\sum_{j=1}^{J} N_j = N$. The observed data can thus be encoded as $X \triangleq \{N_1, \ldots, N_J\}$. Below we describe the implementation of the EM algorithm to estimate $\theta = (\mu, \Sigma)$.

**E-step.** We first express the complete-data log-likelihood as

$$
l(\theta; X, Z) = \sum_{n=1}^{N'} \log f(v_n | \mu, \Sigma). \quad (9)
$$

We then take the expectation of $l(\theta; X, Z)$ conditional on $X$ under the current estimate $\theta^{(t)}$:

$$
Q(\theta | \theta^{(t)}) \triangleq \mathbb{E} \left[ l(\theta; X, Z) \bigg| X, \mu^{(t)}, \Sigma^{(t)} \right]
$$

$$
= \mathbb{E} \left[ \mathbb{E} \left[ \sum_{n=1}^{N'} \log f(v_n | \mu, \Sigma) \bigg| X, \theta^{(t)}, N' \right] \bigg| X, \mu^{(t)}, \Sigma^{(t)} \right]
$$

$$
= \mathbb{E} \left[ \sum_{n=1}^{N'} \int_{v \in R_+^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{x \in R_+^n} f(x | \mu^{(t)}, \Sigma^{(t)}) dx} \log f(v | \mu, \Sigma) dx \bigg| X, \mu^{(t)}, \Sigma^{(t)} \right]. \quad (10)
$$

In the second equation, we first take expectation of the valuations $v_n$ conditional on the total number of customers $N'$ using the tower property. This follows the same derivation as the base model in Section 3.

Next we analyze the distribution $N' | X, \theta^{(t)}$. Note that under $\theta^{(t)}$, a customer is censored with probability $\mathbb{P}(R^0 | \mu^{(t)}, \Sigma^{(t)})$, which represents the probability of the IC polyhedron $R^0$. Therefore, the number
of total customers \( N' \mid \mathbf{X}, \mathbf{\theta}^{(t)} \) can be described by the following probability model: after \( N' \) i.i.d. Bernoulli trials with success probability \( 1 - \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)}) \) (an uncensored customer is counted as a success), there are \( N \) successful trials being observed. Therefore, for \( n = N, N + 1, \ldots \), we have

\[
\mathbb{P} \left( N' = n \mid \mathbf{X}, \mathbf{\theta}^{(t)} \right) = \frac{\mathbb{P} \left( N = m \mid n \mid N' = n \right) \mathbb{P} \left( N' = n \right)}{\mathbb{P} \left( N = m \mid \mathbf{\theta}^{(t)} \right)} = \frac{\mathbb{P} \left( N = m \mid N' = n, \mathbf{\theta}^{(t)} \right) \mathbb{P} \left( N' = n \right)}{\mathbb{P} \left( N = m \right)} = \frac{\mathbb{P} \left( N = m \mid N' = n, \mathbf{\theta}^{(t)} \right) \mathbb{P} \left( N' = n \right)}{\sum_{n=N}^{\infty} \mathbb{P}(N \mid N' = n, \mathbf{\theta}^{(t)}) \mathbb{P}(N' = n)}.
\]

This probability is unspecified unless we have a prior distribution for \( N' \). For this purpose, we use the improper prior following marquis de Laplace (1840) suggesting that one should apply a uniform prior to unknown events from “the principle of insufficient reason”, i.e., \( \mathbb{P}(N' = n_1) = \mathbb{P}(N' = n_2) \) for \( n_1 \neq n_2 \). Therefore, the above term can be expressed as

\[
\frac{\binom{N}{n} \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})^{n-N} \left(1 - \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})\right)^{N-n}}{\sum_{n=N}^{\infty} \binom{N}{n} \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})^{n-N} \left(1 - \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})\right)^{N-n}} = \frac{n!}{N!} \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})^{n-N} \left(1 - \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})\right)^{N+1-\sum_{n=N}^{\infty} \binom{N}{n} \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})^{n-N} \left(1 - \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)})\right)^{N-n}}.
\]

Note that it has the same distribution as the negative binomial distribution with success rate \( 1 - \mathbb{P}(R_0^{(t)}|\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)}) \) and \( N+1 \) successes. Recall that the negative binomial distribution with \( N+1 \) successes describes the probability mass function of the number of trials in independent Bernoulli trials until the \((N+1)\)th success is observed. The use of the improper prior equates the total number of customers to that right before the \((N+1)\)th customer who makes a purchase.

With this formula, we next proceed to (10). Similarly we resort to Monte Carlo simulation in the following steps:

1. Consider \( L \) instances. In instance \( l \), simulate \( N'^{(l)} \) according to the negative binomial distribution (11).
2. Then simulate \( N_j \) samples from \( \mathcal{N}(\mathbf{\mu}^{(t)}, \mathbf{\Sigma}^{(t)}) \) conditional on \( x \in R_0 \), denoted \( \{x^{(l)}_{j,s}\}_{s=1}^{N_j} \), and \( N'^{(l)} - N_j \) samples in \( R_0 \), denoted \( \{x^{(l)}_{0,s}\}_{s=1}^{N'^{(l)}-N_j} \).
3. Approximate the expectation in (10) by

\[
\hat{Q}(\mathbf{\theta}^{(t)}) = \frac{1}{L} \sum_{l=1}^{L} \sum_{j=1}^{N_j} \sum_{s=1}^{N'^{(l)}-N_j} \log f \left( x^{(l)}_{j,s} | \mathbf{\mu}, \mathbf{\Sigma} \right) + \sum_{s=1}^{N'^{(l)}-N_j} \log f \left( x^{(l)}_{0,s} | \mathbf{\mu}, \mathbf{\Sigma} \right).
\]

Note that the information of \( \mathbf{\theta}^{(t)} \) has been fully absorbed by the simulated samples \( N'^{(l)} \) and \( \{x^{(l)}_{j,s}\} \). The formula in (12) is a function of \( (\mathbf{\mu}, \mathbf{\Sigma}) \), which will be optimized in the M-step.

Given \( \hat{Q}(\mathbf{\theta}^{(t)}) \) in (12), the M-step is similar to (7). In particular, \( \mathbf{\mu}^{(t+1)} \) and \( \mathbf{\Sigma}^{(t+1)} \) are the sample mean and variance in the standard MLE for multivariate normal distributions:

\[
\mathbf{\mu}^{(t+1)} = \frac{1}{\sum_{l=1}^{L} N'^{(l)}} \sum_{l=1}^{L} \left( \sum_{j=1}^{N_j} \sum_{s=1}^{N'^{(l)}-N_j} x^{(l)}_{j,s} + \sum_{s=1}^{N'^{(l)}-N_j} x^{(l)}_{0,s} \right),
\]

\[
\mathbf{\Sigma}^{(t+1)} = \frac{1}{\sum_{l=1}^{L} N'^{(l)}} \sum_{l=1}^{L} \left( \sum_{j=1}^{N_j} \sum_{s=1}^{N'^{(l)}-N_j} \left( x^{(l)}_{j,s} - \mathbf{\mu}^{(t+1)} \right) \left( x^{(l)}_{j,s} - \mathbf{\mu}^{(t+1)} \right)^\top \right) + \sum_{s=1}^{N'^{(l)}-N_j} \left( x^{(l)}_{0,s} - \mathbf{\mu}^{(t+1)} \right) \left( x^{(l)}_{0,s} - \mathbf{\mu}^{(t+1)} \right)^\top.
\]

Then Algorithm 2 can be adapted to the censored-demand data.

To conclude this section, we discuss how the EM algorithm can be generalized when customers may observe different price menus provided by the firm, for example, based on the arrival time in a day. Suppose
that the firm offers \( m \) price menus to customers. The transaction data consists of \( N^m \) observed customer purchases from each price menu and their choices. Note that the IC polyhedra differ across the price menus. Using the same procedure stated above, we can use Monte Carlo to simulate the number of total customers \( N^{m,n} \) for each price menu and simulate the valuations of the customers accordingly. They can be used in the M-step to update the parameters.

### 4.2 Gaussian Mixture Models

In this section, we generalize the base model in Section 3 by considering valuation \( v \) of each customer independently drawn from an \( I \)-dimensional Gaussian mixture model with \( K \) components:

\[
v \sim \sum_{k=1}^{K} \phi_k N(\mu_k, \Sigma_k),
\]

where \( \phi_k \geq 0 \) and \( \sum_{k=1}^{K} \phi_k = 1 \) are the mixture proportions, \( N(\mu_k, \Sigma_k) \) is the density of a multivariate Gaussian distribution with mean \( \mu_k \) and covariance matrix \( \Sigma_k \), and \( \theta = (\phi_1, \cdots, \phi_K, \mu_1, \cdots, \mu_K, \Sigma_1, \cdots, \Sigma_K) \) denotes the vector of parameters that we need to estimate. Such a Gaussian mixture model allows for clustering of consumer valuations and can flexibly approximates any distribution.

We use \( \pi^n_k \in \{0, 1\}^K \) to denote the component association of customer \( n \): \( \pi^n_k = 1 \) if \( v_n \) is generated from \( N(\mu_k, \Sigma_k) \) and zero otherwise. Note that in this model, for each transaction there are two missing values: (i) the unobserved valuations, and (ii) the associated component to this valuation. Therefore, the missing data is \( Z \triangleq \{\pi^n_1, \ldots, \pi^n_N, v_1, \ldots, v_N\} \). We express the complete-data log-likelihood function as

\[
l(\theta; X, Z) = \sum_{n=1}^{N} \sum_{k=1}^{K} \pi^n_k [\log(\phi_k) + \log f(v_n | \mu_k, \Sigma_k)],
\]

where recall that \( f(\cdot) \) is the PDF of the multivariate normal distribution.

**E-step.** Since the \( \pi^n_k \) and \( v_n \) are not observed, we consider the expected complete-data log-likelihood. We first compute \( Q(\theta | \theta^{(t)}) \) by computing the expectation of \( l(\theta; X, Z) \) conditional on \( X \) under the current estimate \( \theta^{(t)} \), and thus, we have

\[
Q(\theta | \theta^{(t)}) \triangleq \mathbb{E}_{Z | X, \theta^{(t)}} \left[ l(\theta; X, Z) \bigg| X, \mu^{(t)}, \Sigma^{(t)}, \phi^{(t)} \right]
\]

\[
= \mathbb{E}_{\pi, v | X, \theta^{(t)}} \left[ \sum_{n=1}^{N} \sum_{k=1}^{K} \pi^n_k \log(\phi_k) + \pi^n_k \log f(v_n | \mu_k, \Sigma_k) \bigg| X, \mu^{(t)}, \Sigma^{(t)}, \phi^{(t)} \right]
\]

\[
= \mathbb{E}_{\pi | X, \theta^{(t)}} \left[ \sum_{n=1}^{N} \sum_{k=1}^{K} \pi^n_k \log(\phi_k) + \pi^n_k \log f(v_n | \mu_k, \Sigma_k) \bigg| X, \mu^{(t)}, \Sigma^{(t)}, \phi^{(t)} \right]
\]

\[
= \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{P}(\pi^n_k = 1 | X, \theta^{(t)}) \mathbb{E}[\log(\phi_k) + \log f(v_n | \mu_k, \Sigma_k) | X, \theta^{(t)}, \pi^n_k = 1] \tag{13}
\]

In the last line of (13), we further have

\[
\mathbb{E}[\log f(v_n | \mu_k, \Sigma_k) | X, \theta^{(t)}, \pi^n_k = 1] = \int_{v \in R^{c_n}} \frac{f(v | \mu_k, \Sigma_k)}{\int_{R^{c_n}} f(v | \mu_k, \Sigma_k)dv} \log f(v_n | \mu_k, \Sigma_k)dv.
\]

To calculate (13), we first calculate the probability \( \mathbb{P}(\pi^n_k = 1 | X, \mu^{(t)}, \Sigma^{(t)}, \phi^{(t)}) \), i.e., given the choice \( c_n \) of customer \( n \), what is the probability that \( s/h e \) is associated with component \( k \):

\[
\hat{p}^n_k \triangleq \mathbb{P}(\pi^n_k = 1 | X, \theta^{(t)}) = \frac{\mathbb{P}(R^{c_n} | \mu_k^{(t)}, \Sigma_k^{(t)}, \pi^n_k = 1) \phi^{(t)}_k}{\sum_{k'=1}^{K} \mathbb{P}(R^{c_n} | \mu_{k'}^{(t)}, \Sigma_{k'}^{(t)}, \pi^n_k = 1) \phi^{(t)}_{k'}}. \tag{14}
\]
Note that (14) allows us to directly simulate $\tilde{\pi}_k^n$ for all $k$ and $n$ as an independent subroutine. In particular, given $\theta^{(t)}$, to estimate $\mathbb{P}(R^n | \mu_k^{(t)}, \Sigma_k^{(t)}, \pi_k^n = 1)$, we can generate many Monte Carlo samples from the Gaussian distribution $\mathcal{N}(\mu_k^{(t)}, \Sigma_k^{(t)})$ and record the fraction in $R^n$. As a result, we can use (14) to estimate $\hat{\pi}_k^n$.

Combining this additional step to estimate $\hat{\pi}_k^n$, we can proceed with the EM algorithm for (13):

1. **Estimating $\hat{\pi}_k^n$:** for $k = 1, \ldots, K$, generate $L$ samples $x_k^{(l)}$, $l = 1, \ldots, K$, from $\mathcal{N}(\mu_k^{(t)}, \Sigma_k^{(t)})$. Let

$$\hat{\mathbb{P}}(R^n | \mu_k^{(t)}, \Sigma_k^{(t)}) = \frac{1}{L} \sum_{l=1}^L I \left( x_k^{(l)} \in R^n \right)$$

and plug it into (14) to estimate $\hat{\pi}_k^n$.

2. For all observations $n = 1, \ldots, N$ and $K$ components $k = 1, \ldots, K$, generate $L$ samples $x_{nk}^{(l)}$, $l = 1, \ldots, L$ from $\mathcal{N}(\mu_k^{(t)}, \Sigma_k^{(t)})$ conditional on $x_{nk}^{(l)} \in R^n$, using Algorithm 1.

3. **E-step:** We represent (13) as

$$\sum_{n=1}^N \sum_{k=1}^K \hat{\pi}_k^n \log(\phi_k) + \frac{1}{L} \sum_{l=1}^L \sum_{n=1}^N \sum_{k=1}^K \hat{\pi}_k^n \log f(x_{nk}^{(l)} | \mu_k, \Sigma_k).$$

4. **M-step:** from the first term in (15) we can maximize $\phi_k$ for $k = 1, \ldots, K$:

$$\phi_k^{(t+1)} = \sum_{n=1}^N \frac{1}{N} \hat{\pi}_k^n.$$

For the mean and variance, we have

$$\mu_k^{(t+1)} = \frac{\sum_{l=1}^L \sum_{n=1}^N \hat{\pi}_k^n x_{nk}^{(l)}}{\sum_{n=1}^N \hat{\pi}_k^n},$$

$$\Sigma_k^{(t+1)} = \frac{\sum_{l=1}^L \sum_{n=1}^N \hat{\pi}_k^n (x_{nk}^{(l)} - \mu_k^{(t+1)}) (x_{nk}^{(l)} - \mu_k^{(t+1)})^\top}{\sum_{n=1}^N \hat{\pi}_k^n}.$$

5. We repeat the above steps until the parameters converge.

### 5 Theoretical Properties

In this section, we present the statistical properties of the base model in Section 3 and the EM algorithm. We first establish conditions for the identifiability of the problem. We then show some properties of the convergence of the EM algorithm.

#### 5.1 Identifiability

The identifiability is concerned with the notion that whether the parameter $\theta = (\mu, \Sigma)$ can ever be learned from the data. For example, suppose the firm has collected a large data set after keeping the price menu for a long period. Equivalently, the probabilities of the IC polyhedra in (4) can be accurately estimated, from the fraction of customers purchasing each bundle. Identifiability guarantees that knowing the probability of the regions (IC polyhedra) uniquely determines the parameters.

To simplify the notation and formulate the problem in a way of independent theoretical interest, consider a class of regions $\mathcal{R} \triangleq \{R_1, \ldots, R_K\}$ where $R_k \subset \mathbb{R}^I$. The identifiability of our model is defined as
Definition 1 (Identifiability) For a family of multivariate normal distribution in $\mathbb{R}^I$
\[ P = \left\{ f(v|\theta) = \frac{1}{\sqrt{(2\pi)^I|\Sigma|}} \exp \left( -\frac{1}{2} (v - \mu)\Sigma^{-1}(v - \mu) \right) \mid \theta = (\mu, \Sigma) \right\}, \]
we say that the model is identifiable over $\mathcal{R}$ if we have
\[
\int_{v \in R_i} f(v|\theta)dv = \int_{v \in R_i} f(v|\theta)dv \quad \text{for all } R_i \in \mathcal{R} \implies \theta_1 = \theta_2.
\]

In other words, for the collection of IC polyhedra $\mathcal{R}$ represented by two regions (intervals): $R_1 = (-\infty, 10)$ and $R_2 = [10, +\infty)$. The model is not identifiable because $\theta_1$ and $\theta_2$ satisfying $(\mu_1 - 10)/\sigma_1 = (\mu_2 - 10)/\sigma_2$ always lead to the same probability $P(R_1|\theta_1) = P(R_1|\theta_2)$ and $P(R_2|\theta_1) = P(R_2|\theta_2)$.

Therefore, we need to establish conditions for $\mathcal{R}$ that guarantee identifiability. Intuitively, since there are $K$ regions and $(I + 1)^2/2$ effective parameters in the model, we require $K \geq (I + 1)^2/2$. However, because of the nonlinearity in the probabilities of the regions, it is hard to verify the sufficiency or the necessity of this condition.

Based on the application, we provide the following sufficient condition that can be easily satisfied in practice. Suppose the firms are selling products separately. Technically, the firm determines the prices for the $I$ individual prices and offering $J = 2^I$ bundles; the price of a bundle $J$ is the sum of the prices of the included individual products. Separate selling is prevalent in retailing, when firms don’t bundle products together.

Proposition 1 (Identifiability under separate selling) When the firm sells products separately, as long as at least two prices are set for each individual products infinitely often, then the model is identifiable.

Note that Proposition 1 does not require all combinations of the two prices of the products to be offered infinitely often, which would result in $2^I$ price menus. Instead, a simple and realistic scenario with $I + 1$ price menus would suffice: a price menu of regular prices of the products $(p_1, \ldots, p_I)$ and $J$ price menus in which only one product is on discount, i.e., $(p_1, \ldots, p_{i-1}, p_i', p_{i+1}, \ldots, p_I)$ for product $i$. If the above $I + 1$ price menus are offered infinitely often, then $\mathcal{R}$ includes the following regions, whose probabilities turn out to be sufficient for identifiability:
\[
\begin{align*}
\{v \in \mathbb{R}^I, v_1 \leq p_1\}, \{v \in \mathbb{R}^I, v_i \leq p_i\}, & \quad \forall i = 1, \ldots, I \\
\{v \in \mathbb{R}^I, v_{i_1} \leq p_{i_1}, v_{i_2} \leq p_{i_2}\}, \{v \in \mathbb{R}^I, v_{i_1} \leq p'_{i_1}, v_{i_2} \leq p'_{i_2}\} & \quad \forall i_1, i_2 = 1, \ldots, I
\end{align*}
\]
By Example 2, just setting one price for a product is not sufficient for identifiability. Therefore, Proposition 1 provides a sufficient and necessary condition for identifiability under separate selling.

5.2 Convergence of the EM Algorithm

The EM algorithm has been shown to converge to a local maximum of the likelihood function in the seminal papers by Dempster et al. (1977), Wu (1983). However, the convergence to the global maximum of the likelihood function, which corresponds to the true parameters with large samples, remains an active research
area. The new theoretical advances Balakrishnan et al. (2017) in the study of EM algorithms allow one to characterize the conditions for the convergence to the global maximum of the likelihood function. In this section, we use the approach in Balakrishnan et al. (2017) to analyze our problem. To simplify the analysis, we focus on the population-level $Q$-function, following the first step in Balakrishnan et al. (2017). That is, the EM algorithm is run on a dataset with an infinite sample size. We also assume the IC polyhedra are identical for all consumers, i.e., they face the same price menu. As a result, we can focus on a partition of $\mathbb{R}^n$, denoted $\{R_k\}_{k=1}$. Moreover, we assume the true $\Sigma^*$ is known and the EM algorithm finds the maximum likelihood estimator for $\mu$. The $Q$-function in this simplified setting can be expressed as

$$Q(\mu' | \mu) = \sum_{k=1}^{K} \int_{x \in R_k} f(x | \mu') dx \int_{v \in R_k} \frac{f(v | \mu)}{\int_{x \in R_k} f(x | \mu) dx} \log f(v | \mu') dv.$$  \hspace{1cm} (16)

Compared to (6), we remove the dependence on $\Sigma$ and use the same partition. Moreover, because the function is defined at the population level, the probability $\int_{x \in R_k} f(x | \mu')$ in each region replaces the samples in (6). The population-level EM algorithm updates $\mu$ iteratively according to the following operator:

$$M(\mu) \triangleq \arg\max_{\mu'} Q(\mu' | \mu).$$

More precisely, given initialization $\mu^{(0)}$, the EM algorithm uses $\mu^{(t+1)} = M(\mu^{(t)})$ to obtain a sequence $\{\mu^{(t)}\}_{t=0}^{\infty}$. The theoretical question is whether we have $\mu^{(t)} \rightarrow \mu^*$. Note that the true value $\mu^*$ always maximizes the population-level likelihood function (Van der Vaart 2000). Moreover, it satisfies the self-consistency condition (McLachlan and Krishnan 2007): $\mu^* = \arg\max_{\mu'} Q(\mu' | \mu^*)$. Therefore, $\mu^*$ is a fixed point of $M(\mu) = \mu$. Balakrishnan et al. (2017) establish a set of conditions that guarantee $M(\mu)$ to be a contraction mapping when $\mu^{(0)}$ is in a neighborhood of $\mu^*$, denoted by $B(r; \mu^*)$ with an Euclidean radius $r$. Since the contraction mapping converges to the fixed point, our goal in this section is to verify the set of conditions in our problem.

Among the set of technical conditions in Balakrishnan et al. (2017), there are two key conditions relevant to our model:

- **Concavity of $Q(\mu | \mu^*)$.** Define $q(\mu) \triangleq Q(\mu | \mu^*) = \sum_{k=1}^{K} \int_{v \in R_k} f(v | \mu^*) \log f(v | \mu) dv$ as the $Q$-function when the current $\mu$ is the true value $\mu^*$. The required condition states that there exists $\lambda > 0$, such that

$$q(\mu_1) - q(\mu_2) - \langle \nabla q(\mu_2), \mu_1 - \mu_2 \rangle \leq -\frac{\lambda}{2} \|\mu_1 - \mu_2\|^2,$$  \hspace{1cm} (17)

for all pairs of $\mu_1, \mu_2 \in B(r; \mu^*)$, where $\nabla$ is the gradient operator of a function. Represented in the Taylor expansion, (17) ensures that $q(\mu)$ is strictly concave when $\mu$ is in the neighborhood.

- **First-order stability.** Note that $\nabla Q(\mu' | \mu)$ is the gradient of $Q$ at $\mu'$ given the current $\mu$. This condition requires that for some $\gamma < \lambda$, we have

$$\|\nabla Q(M(\mu) | \mu^*) - \nabla Q(M(\mu) | \mu)\|_2 \leq \gamma \|\mu - \mu^*\|_2.$$  \hspace{1cm} (18)

In other words, the $Q$-function needs to be sufficiently stable around $\mu^*$ when taking the gradient. The relationship $\gamma < \lambda$ is essential, as $\gamma/\lambda$ turns to be the contraction constant.

Note that neither condition can be easily checked in our model. The main contribution of this section is to identify reasonable assumptions for the conditions to hold.

Let $X \sim \mathcal{N}(\mu^*, \Sigma^*)$ be the distribution of the valuation and $Z = (\Sigma^*)^{-1/2}(X - \mu^*)$ be the linear transformation of $X$ so that $Z \sim \mathcal{N}(0, I)$. Let $R_k^* = (\Sigma^*)^{-1/2}(R_k - \mu^*)$ be the transformed regions in the $Z$ space. Therefore, $\mathbb{E}[Z | R_k^*]$ is the conditional expectation of $Z$ in $R_k^*$. We let $R'$ be a categorical random variable so that $\mathbb{P}(R' = R_k^*) = \mathbb{P}(Z \in R_k^*)$. The assumption below provides a sufficient condition for the EM algorithm to converge. We use $\lambda_{\min}(\cdot)$ to denote the minimal eigenvalue of a positive semi-definite matrix.

**Assumption 1** $\lambda_{\min}(\text{Var}(\mathbb{E}[Z | R'])) \geq \epsilon$ for some $\epsilon > 0$. 

Note that \(\mathbb{P}(\mathbb{E}[Z \mid R'] = \mathbb{E}[Z \mid R'_k]) = \mathbb{P}(Z \in R'_k)\) and thus \(\mathbb{E}(Z \mid R')\) is an \(I\)-dimensional random vector supported on \(K\) points. Assumption 1 states that the eigenvalues of the covariance matrix of the random vector are bounded away from zero.

To provide some intuition for the assumption, consider the case \(K = 1\), i.e., there is one region. In this case, \(\mathbb{E}(Z \mid R')\) has a single value and \(\text{Var}(\mathbb{E}[Z \mid R'])\) is a degenerate \(I \times I\) zero matrix. Assumption 1 is clearly not satisfied. It is not surprising that the EM algorithm doesn’t converge to the true parameters for this degenerate case because the model is not identifiable, i.e., no information about the parameters can be learned from the data.

Now consider the other extreme. Suppose \(R'_k\) partitions the space extremely finely so that \(R'_k\) almost degenerates to a single point. In this case, \(\mathbb{E}[Z \mid R']\) is itself approximately \(N(0, I)\). Therefore, \(\text{Var}(\mathbb{E}[Z \mid R']) \approx I\) and apparently satisfies Assumption 1. The two examples point to the intuition that the EM algorithm performs well when there are many small regions. This is consistent with the intuition mentioned after Example 2.

Assumption 1 guarantees the convergence of the EM algorithm to the true parameter locally.

**Theorem 1** Suppose Assumption 1 holds. There exists a neighborhood \(\mathbb{B}(r; \mu^*)\) of \(\mu^*\) such that for \(\mu^{(0)} \in \mathbb{B}(r; \mu^*)\) the EM algorithm guarantees

\[
\|\mu^{(t)} - \mu^*\|_2 \leq (1 - \epsilon/2)^t \|\mu^{(0)} - \mu^*\|_2.
\]

The detailed proof for Theorem 1 can be found in the online appendix.

### 6 Numerical Experiments

In this section, we conduct the numerical experiments to study the performance of the EM algorithm. Because there are few methods that can be applied to bundle sales data, our main benchmark is an adapted MNL model, treating each bundle as an individual product. We also implement the algorithm in Jedidi et al. (2003).

We generate multiple synthetic datasets with \(I = 2, 4, 6\) products and \(N = 1000, 2000, 4000\) transactions. Each transaction records a customer’s consideration set, their prices and the customer’s choice (including no-purchase). Customers’ consideration set is randomly drawn with probability 0.5 from the product set and also includes random bundles of sizes 2 and 3, consisting of the products viewed by the customer. We consider that prices for individual products following a uniform distribution \([\mu_i - 3, \mu_i + 3]\), where \(\mu_i\) denote the mean of the valuation distribution for product \(i\). For bundles, we get the summation of individual prices within the bundle and generate a discount from a uniform distribution \([0, 5]\). For example, consider a bundle including products \(\{1, 2, 3\}\), with respective prices 10, 20, 30. If the random discount is 2, then the bundle price is \(10 + 20 + 30 - 2 = 58\). For the ground truth, we consider two underlying demand models: Gaussian distribution, where its mean is drawn from a uniform distribution \(\mu \sim U[10, 50]^I\), and the covariance matrix is \(\Sigma = AA^\top\), where the component of \(A\) follows \(U[1, 2]\); Gumbel distribution, where we consider an independent Gumbel distribution for each product \(i\) with parameters \(\mu\) and the diagonals of \(\Sigma\). We use an additive function to evaluate customers’ valuation for bundles.

#### 6.1 The Base Model

In this subsection, we compare the performance of the EM algorithm with the MNL model treating each bundle accounts as a different/separate product. We use 80% of our dataset for training and the remaining 20% for testing the model prediction. We measure the estimation by the \(\ell_1\)-error \((\|\mu^{(t+1)} - \mu^*\|_1 + \|\Sigma^{(t+1)} - \Sigma^*\|_1)/(K^2 + K)\) which is the average absolute difference of the estimated component and the true parameter.

**EM convergence.** Figure 1 depicts the error of the EM algorithm over the iterations. Figure 1(a) shows that the EM algorithm almost recovers the true parameters (i.e., \(\text{error} < 0.1\)) in 15 iterations. Figure 1(b) demonstrates that the more products or transactions, the lower the error, and the faster the algorithm converges to the true parameters.

**EM vs. MNL.** In Figure 2, we measure the performance of the EM algorithm and the adapted MNL model in terms of root-mean square error (RMSE). This is because we cannot evaluate the error against
EM vs. Hierarchical Bayesian Model. In this experiment, we compare the efficacy of the proposed EM algorithm with the approach in Jedidi et al. (2003), in which they form a multinomial probit likelihood which involves integration over high-dimensional multivariate normal distribution, and propose a hierarchical Bayesian method to infer the parameters based on the posterior distribution using Metropolis Hasting method. We implement their method in our setting by considering the posterior probability $P(\mu^{(t)}, \sigma^{(t)} | R^n) \propto P(R^n | \mu^{(t)}, \sigma^{(t)}) P(\mu^{(t)}) P(\sigma^{(t)})$ (see the Metropolis Hasting algorithm in Appendix B.3). We run this model for two products with fixed covariance matrix $\begin{bmatrix} 4 & 1 \\ 1 & 5 \end{bmatrix}$. We generate 1000 random observations with mean $[\mu_1, \mu_2] = [0.5, 0.5]$. Our EM algorithm converges to $[0.562, 0.588]$ after 20 iterations in 2.368 minutes, which implies an error of 0.075. For the Metropolis Hasting algorithm, we iterate the
model 10000 times for about 7 days, and it converges to $[0.391, 0.685]$, with an error 0.147. This shows the advantage of our model over the Metropolis Hasting algorithm to infer the true parameters.

6.2 Censored Data

In this subsection, we show the efficacy of our model to recover true parameters when no-purchases are censored from the sales data and there is no record of such transactions. In this experiment, we randomly generate a complete dataset (including no-purchase transactions) with $I = 2, 4, 6$ products and $N = 1000, 2000, 4000$ transactions as explained in Subsection 6.1 with an exception that the number of observation sets, price menus and bundles are limited to 1, 3, and 6. As explained in Section 4.1, we need the seller to collect data for the same price menu in order to estimate the model from censored demand. This is why we use a smaller number of price menus than the experiments for the base model.

We perform the base EM algorithm on the complete dataset and then, we remove the no-purchase transactions (approx. 5-15% of the transactions) and perform the EM algorithm for censored data. Figure 3(a) shows that the EM algorithm for censored data converges, and the error is less when the number of transactions increases. Moreover, we have that the difference between the RMSE of complete and censored datasets is less than 0.002 (0.6%).

Fig. 3. EM censored performance EM censored for 4 products, 3 bundles, and 3 price menus
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Online Appendix

A Proofs

A.1 The Derivation of the M-step

Thus, we have

\[ Q \left( \theta | \theta^{(t)} \right) \triangleq \mathbb{E} \left[ l(\theta; X, Z) \mid X, \mu^{(t)}, \Sigma^{(t)} \right] = \sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \log f(v | \mu, \Sigma) \, dv. \]  \tag{A.1}

To find a new estimation for \( \theta \), the M-step in the EM algorithm maximizes \( Q \left( \theta | \theta^{(t)} \right) \) and let \( \theta^{(t+1)} = \arg\max_{\theta} Q \left( \theta | \theta^{(t)} \right) \). Thus, we first solve

\[ \frac{\partial}{\partial \mu} \mathbb{E} \left[ l(\theta; X, Z) \mid X, \mu^{(t)}, \Sigma^{(t)} \right] / \partial \mu = 0, \]  \tag{A.2}

and then we solve

\[ \frac{\partial}{\partial \Sigma} \mathbb{E} \left[ l(\theta; X, Z) \mid X, \mu^{(t)}, \Sigma^{(t)} \right] / \partial \Sigma = 0. \]  \tag{A.3}

Equality (A.2) equates to

\[
\begin{align*}
\frac{\partial}{\partial \mu} \mathbb{E} \left[ l(\theta; X, Z) \mid X, \mu^{(t)}, \Sigma^{(t)} \right] & = \frac{\partial}{\partial \mu} \sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \log f(v | \mu, \Sigma) \, dv \\
& = \sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \frac{\partial}{\partial \mu} \log f(v | \mu, \Sigma) \, dv \\
& = \sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \frac{\partial}{\partial \mu} f(v | \mu, \Sigma) \Sigma^{-1}(v - \mu) f(v | \mu, \Sigma) \, dv \\
& = \sum_{n=1}^{N} \int_{R^n} \frac{\Sigma^{-1}(v - \mu)}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \, dv \\
& = \sum_{n=1}^{N} \frac{\int_{R^n} f(v | \mu^{(t)}, \Sigma^{(t)}) \, dv}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} - \sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \, dv \\
& = \sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \, dv - N \mu = 0. \tag{A.4}
\end{align*}
\]

Thus, we have

\[
\mu = \frac{\sum_{n=1}^{N} \int_{R^n} \frac{f(v | \mu^{(t)}, \Sigma^{(t)})}{\int_{R^n} f(x | \mu^{(t)}, \Sigma^{(t)}) \, dx} \, dv}{N} = \frac{\sum_{n=1}^{N} \mathbb{E}[v | \mu^{(t)}, \Sigma^{(t)}, R^n_n]}{N}. \tag{A.5}
\]
Proof of Proposition 1: We prove the result using induction on $I$.

**Identifiability**

Suppose product one is offered at at least two prices $p_1 < p_1'$. It implies the probabilities of the regions $R' = \{v \in \mathbb{R}^{I+1}; v_1 \leq p_1\}$ (the fraction of customers who have bought product one at price $p_1$) and
\[ R'' = \{ v \in \mathbb{R}^{I+1}, v_1 \leq p'_1 \} \] are determined. By the argument in the base case, we can uniquely determine \( \mu_1 \) and \( \sigma_{11} \).

Now it remains to show that \( \sigma_{1k} = \sigma_{k1} \) for \( k = 2, \ldots, I + 1 \) can be uniquely determined. Without loss of generality, we focus on \( \sigma_{12} \). Suppose product two is offered at two prices \( p_2 \) and \( p'_2 \). Since products one and two are offered together, one of the combinations of their individual prices, \((p_1, p_2), (p_1, p'_2), (p'_1, p_2)\) and \((p'_1, p'_2)\), must have been offered infinitely in the data. Without loss of generality, suppose \((p_1, p_2)\) is offered. It implies the probability of the following region is determined:

\[ R_1 = \{ v \in \mathbb{R}^{I+1}, v_1 \geq p_1, v_2 \geq p_2 \}, \quad R_2 = \{ v \in \mathbb{R}^{I+1}, v_1 \leq p_1, v_2 \leq p_2 \}. \]

Indeed, the probability of \( R_1 (R_2) \) is the fraction of customers who bought both (neither) products when they are offered at \( p_1 \) and \( p_2 \), respectively. Note that the joint distribution of \((V_1, V_2)\) is Gaussian with mean \((\mu_1, \mu_2)\) and covariance matrix \([\sigma_{11}, \sigma_{12}; \sigma_{12}, \sigma_{22}]\), all of which are uniquely determined but \( \sigma_{12} \). It remains to show that \( \sigma_{12} \) is also uniquely determined by \( \mathbb{P}(R_1) \) and \( \mathbb{P}(R_2) \).

For this purpose, without loss of generality, for the simplicity of notations, we assume \( \mu_1 = \mu_2 = 0 \) and \( \sigma_{11} = \sigma_{22} = 1 \). In this case, \( \sigma_{12} \in [-1, 1] \) is the correlation of \( V_1 \) and \( V_2 \). We next prove the result by contradiction. That is, suppose there exist \( \sigma_{12} \neq \sigma'_{12} \) such that \( \mathbb{P}(R_1|\sigma_{12}) = \mathbb{P}(R_1|\sigma'_{12}) \) and \( \mathbb{P}(R_2|\sigma_{12}) = \mathbb{P}(R_2|\sigma'_{12}) \). Consider the following two linear transformations of \((V_1, V_2)\):

\[
T : (X_1, X_2) = \left( V_1, -\frac{\sigma_{12}}{\sqrt{1-\sigma_{12}^2}} V_1 + \frac{1}{\sqrt{1-\sigma_{12}^2}} V_2 \right)
\]

\[
T' : (X'_1, X'_2) = \left( V_1, -\frac{\sigma'_{12}}{\sqrt{1-\sigma_{12}^2}} V_1 + \frac{1}{\sqrt{1-\sigma_{12}^2}} V_2 \right).
\]

Note that both transformations keep \( V_3, \ldots, V_{I+1} \) unchanged, which don’t play a role in the subsequent proof. It is easy to verify that \( X_1 \) and \( X_2 \) are independent standard normal random variables if the correlation between \( V_1 \) and \( V_2 \) is \( \sigma_{12} (\sigma'_{12}) \). We next consider the transformed region of \( R_1 \) under \( T' \):

\[
T(R_1) = \{ x \in \mathbb{R}^{I+1}, x_1 \geq p_1, \sigma_{12} x_1 + \sqrt{1-\sigma_{12}^2} x_2 \geq p_2 \}.
\]

The transformed region of \( R_2 \) and both transformed regions under \( T' \) can be defined analogously, by replacing \( \sigma_{12} \) by \( \sigma'_{12} \). We consider the two lines of \( \mathbb{R}^2: \sigma_{12} x_1 + \sqrt{1-\sigma_{12}^2} x_2 = p_2 \) and \( \sigma'_{12} x_1 + \sqrt{1-\sigma_{12}^2} x_2 = p_2 \). Because \( \sigma_{12} \neq \sigma'_{12} \), it is easy to show that \( \sigma_{12}/\sqrt{1-\sigma_{12}^2} \neq \sigma'_{12}/\sqrt{1-\sigma_{12}^2} \). As a result, the two lines are not parallel and intersect at, say, \((a_1, a_2)\). Without loss of generality, suppose the first line is always on top when \( x_1 < a_1 \), i.e.,

\[
\frac{1}{\sqrt{1-\sigma_{12}^2}}(p_2 - \sigma_{12} x_1) > \frac{1}{\sqrt{1-\sigma_{12}^2}}(p_2 - \sigma'_{12} x_1) \tag{A.8}
\]

for \( x_1 < a_1 \) and vice versa for \( x_1 > a_1 \). If \( a_1 \geq p_1 \), then for \((x_1, x_2, \ldots, x_{I+1}) \in T'(R_2) \), we have

\[
(x_1, x_2, \ldots, x_{I+1}) \in T'(R_2) \Rightarrow x_1 \leq p_1, x_2 \leq \frac{1}{\sqrt{1-\sigma_{12}^2}}(p_2 - \sigma'_{12} x_1)
\]

\[
\Rightarrow x_1 \leq p_1, x_2 \leq \frac{1}{\sqrt{1-\sigma_{12}^2}}(p_2 - \sigma_{12} x_1)
\]

\[
\Rightarrow (x_1, x_2, \ldots, x_{I+1}) \in T(R_2).
\]

The second line is due to (A.8) and the fact that \( x_1 \leq p_1 \leq a_1 \). It implies that \( T'(R_2) \subset T(R_2) \). Moreover, because (A.8) holds strictly, we can find point such as that is in \( T(R_2) \) but not in \( T'(R_2) \). Therefore, \( T'(R_2) \subsetneq T(R_2) \). This leads to a contradiction because

\[
\mathbb{P}(\{V_1, V_2, V_3, \ldots, V_{I+1}\} \in R_2|\sigma_{12}) = \mathbb{P}(\{X'_1, X'_2, V_3, \ldots, V_{I+1}\} \in T'(R_2))
\]

\[
< \mathbb{P}(\{X_1, X_2, V_3, \ldots, V_{I+1}\} \in T(R_2)) = \mathbb{P}(\{V_1, V_2, V_3, \ldots, V_{I+1}\} \in R_2|\sigma_{12}),
\]

which contradicts the fact that \( R_2 \) has the same probability under \( \sigma_{12} \) and \( \sigma'_{12} \). The inequality is due to the fact that \((X_2, X_2)\) and \((X'_1, X'_2)\) have the same normal distribution and the fact that \( T'(R_2) \subset T(R_2) \).

If \( a_1 < p_1 \), we can obtain a similar contradiction by focusing on \( T(R_1) \) and \( T'(R_1) \). This shows that the probability of \( R_1 \) and \( R_2 \) uniquely determines \( \sigma_{12} \), and we have completed the inductive step.
B Proofs for Section 5.2: EM Convergence

B.1 Preliminaries

Recall the definition of the population-level Q-function:

\[
Q(\mu' | \mu) = \sum_{k=1}^{K} \left( \int_{x \in R_k} f(x|\mu') dx \right) \int_{v \in R_k} \frac{f(v | \mu)}{\int_{x \in R_k} f(x|\mu) dx} \log f(v | \mu') dv.
\]  (B.1)

By definition \(q(M(\mu)) = Q(M(\mu) | \mu^*)\), we have

\[
q(M(\mu)) = Q(M(\mu) | \mu^*) = \sum_{k=1}^{K} \int_{v \in R_k} f(v | \mu^*) \log f(v | M(\mu)) dv = \mathbb{E}_{\mu^*} [\log f(v | M(\mu))]
\]  (B.2)

Moreover, \(Q(M(\mu) | \mu)\) is equal to

\[
Q(M(\mu) | \mu) = \sum_{k=1}^{K} \left( \int_{x \in R_k} f(x|\mu^*) dx \right) \int_{v \in R_k} \frac{f(v | \mu)}{\int_{x \in R_k} f(x|\mu) dx} \log f(v | M(\mu)) dv
\]

\[
= \sum_{k=1}^{K} \left( \int_{x \in R_k} f(x|\mu^*) dx \right) \int_{v \in R_k} f(v | \mu) \log f(v | M(\mu)) dv
\]  (B.3)

To take the gradients of \(q(\mu) = Q(\mu | \mu^*)\) and \(Q(\mu | \mu)\), note that

\[
\nabla \log f(v | \mu) = (\Sigma^*)^{-1}(v - \mu)
\]

by the PDF of the Gaussian distribution. Therefore,

\[
\nabla Q(M(\mu) | \mu) = \sum_{k=1}^{K} \left( \int_{x \in R_k} f(x|\mu^*) dx \right) \int_{v \in R_k} f(x | \mu)(\Sigma^*)^{-1}(x - M(\mu)) dx
\]

\[
= \sum_{k=1}^{K} \left( \int_{x \in R_k} f(x|\mu^*) dx \right) \left( \int_{v \in R_k} f(x | \mu)(\Sigma^*)^{-1} x dx - \int_{v \in R_k} f(v | \mu) dv(\Sigma^*)^{-1} M(\mu) \right)
\]

\[
= \sum_{k=1}^{K} \left( \int_{x \in R_k} f(x|\mu^*) dx \right) \int_{v \in R_k} f(x | \mu)(\Sigma^*)^{-1} x dx - (\Sigma^*)^{-1} M(\mu)
\]  (B.4)

\[
\nabla q(\mu) = \mathbb{E}_{\mu^*} [(\Sigma^*)^{-1}(x - \mu)] = (\Sigma^*)^{-1}(\mu^* - \mu)
\]  (B.5)

B.2 EM Convergence

Lemma B.1 For all \(\mu_1, \mu_2\), we have

\[
q(\mu_1) - q(\mu_2) - \langle \nabla q(\mu_2), \mu_1 - \mu_2 \rangle \leq -\frac{1}{2\lambda_{\min}(\Sigma^*)} \|\mu_1 - \mu_2\|_2^2.
\]

Proof. Proof of Lemma B.1: Expanding the left-hand side, we have

\[
q(\mu_1) - q(\mu_2) - \langle \nabla q(\mu_2), \mu_1 - \mu_2 \rangle
\]

\[
= \mathbb{E}_{\mu^*} [\log f(x | \mu_1)] - \mathbb{E}_{\mu^*} [\log f(x | \mu_2)] - \langle (\Sigma^*)^{-1}(\mu^* - \mu_2), \mu_1 - \mu_2 \rangle
\]  (B.6)

\[
= \mathbb{E} \left[ -\frac{1}{2} (x - \mu_1)^T (\Sigma^*)^{-1} (x - \mu_1) \right] - \mathbb{E} \left[ -\frac{1}{2} (x - \mu_2)^T (\Sigma^*)^{-1} (x - \mu_2) \right] - \langle (\Sigma^*)^{-1}(\mu^* - \mu_2), \mu_1 - \mu_2 \rangle
\]

\[
= \frac{1}{2} (\mu_1 - \mu_2)^T (\Sigma^*)^{-1} (\mu_1 - \mu_2),
\]
where (B.6) follows from (B.2), and (B.5). Thus, we have
\[
q(\mu_1) - q(\mu_2) - (\nabla q(\mu_2), \mu_1 - \mu_2) \leq \frac{\| (\Sigma^*)^{-1} \|_2}{2} \| \mu_1 - \mu_2 \|_2,
\]
by the definition of the 2-norm of a matrix. Note that \( \| (\Sigma^*)^{-1} \|_2 = \lambda_{max}(\Sigma^*)^{-1} = \lambda_{min}(\Sigma^*)^{-1}, \)
where \( \lambda_{max}(\cdot) \) and \( \lambda_{min}(\cdot) \) are the maximum and minimum eigenvalues of a matrix. This proves the result of Lemma B.1.

**Lemma B.2** Suppose Assumption 1 holds. We can find a neighborhood \( B_2(r; \mu^*) \) such that for \( \mu \in B_2(r; \mu^*) \) we have
\[
\| \nabla Q(M(\mu) \mid \mu) - \nabla Q(M(\mu) \mid \mu^*) \|_2 \leq \frac{(1 - \epsilon/2)}{\lambda_{min}(\Sigma^*)} \| \mu - \mu^* \|_2.
\]

**Proof.** Proof of Lemma B.2. Using (B.4), we have
\[
\nabla Q(M(\mu) \mid \mu^*) - \nabla Q(M(\mu) \mid \mu)
= -(\Sigma^*)^{-1}(\mu^* - M(\mu)) + \sum_{k=1}^{K} \int_{x \in R_k} f(x | \mu^*) dx \int_{x \in R_k} f(v | \mu)(\Sigma^*)^{-1}vdv - (\Sigma^*)^{-1}M(\mu)
= (\Sigma^*)^{-1} \left( \sum_{k=1}^{K} \int_{x \in R_k} f(x | \mu^*) dx \int_{x \in R_k} f(x | \mu) dx \right) \left( \int_{x \in R_k} f(x | \mu) dx \right)^{-1}
\]
We next use the Taylor expansion on the above quantity. To do so, we first derive the gradient of \( g_k(\mu) \equiv \int_{R_k} f(x | \mu) dx \)
\[
\nabla g_k(\mu) = \frac{\int_{x \in R_k} x(\nabla f(x | \mu))^\top dx \int_{x \in R_k} f(x | \mu) dx - \int_{x \in R_k} f(x | \mu) dx \int_{x \in R_k} (\nabla f(x | \mu))^\top dx}{\left( \int_{R_k} f(x | \mu) dx \right)^2}
\]
\[
= \left( \int_{R_k} x(x - \mu)^\top (\Sigma^*)^{-1} f(x | \mu) dx \right) \left( \int_{R_k} f(x | \mu) dx \right) \left( \int_{R_k} f(x | \mu) dx \right)^{-1} \left( \int_{R_k} f(x | \mu) dx \right)\]
\[
- \left( \int_{R_k} f(x | \mu) dx \right) \left( \int_{R_k} x(x - \mu)^\top (\Sigma^*)^{-1} f(x | \mu) dx \right) \left( \int_{R_k} f(x | \mu) dx \right)^{-1} \left( \int_{R_k} f(x | \mu) dx \right)\]
\[
= \left( \int_{R_k} (x - \mu)^\top (\Sigma^*)^{-1} f(x | \mu) dx \right) \left( \int_{R_k} f(x | \mu) dx \right) \left( \int_{R_k} f(x | \mu) dx \right)^{-1} \left( \int_{R_k} f(x | \mu) dx \right)\]
\[
- \left( \int_{R_k} f(x | \mu) dx \right) \left( \int_{R_k} (x - \mu)^\top (\Sigma^*)^{-1} f(x | \mu) dx \right) \left( \int_{R_k} f(x | \mu) dx \right)^{-1} \left( \int_{R_k} f(x | \mu) dx \right)\]
\[
= \left( \mathbb{E}_\mu [(X - \mu)(X - \mu)^\top | R_k] - (\int_{R_k} (x - \mu)f(x | \mu) dx) \left( \int_{R_k} f(x | \mu) dx \right)^{-1} \left( \int_{R_k} f(x | \mu) dx \right)\right) \left( \Sigma^* \right)^{-1}\]
\[
= \left( \mathbb{E}_\mu ((X - \mu)X^\top | R_k] - \mathbb{E}_\mu [X | R_k]|\mathbb{E}_\mu [X - \mu | R_k]^\top \right) \left( \Sigma^* \right)^{-1}\]
\[
= \text{Var}_\mu (R_k) \left( \Sigma^* \right)^{-1}.
\]
In the last line, we use \( \text{Var}(R_k|\mu) \) to denote the covariance matrix of the conditional distribution of \( N(\mu, \Sigma^*) \) in the region \( R_k \). Therefore, by the Taylor expansion, we have

\[
\nabla Q(M(\mu) | \mu) - \nabla Q(M(\mu) | \mu^*)
= (\Sigma^*)^{-1} \sum_{k=1}^{K} \int_{x \in R_k} f(x|\mu^*) dx \nabla g_k(\mu^*)(\mu - \mu^*) + O(\|\mu^* - \mu\|_2^2)
= (\Sigma^*)^{-1} \sum_{k=1}^{K} \int_{x \in R_k} f(x|\mu^*) dx \text{Var}_{\mu^*}(R_k)(\Sigma^*)^{-1}(\mu - \mu^*) + O(\|\mu^* - \mu\|_2^2).
\]

(B.10)

Note that if we interpret \( R \) as a categorical random variable, with \( P(R = R_k) = \sum_{k=1}^{K} \int_{x \in R_k} f(x|\mu^*) dx \), then by the law of total covariance we have

\[
\sum_{k=1}^{K} \int_{x \in R_k} f(x|\mu^*) dx \text{Var}(R_k) = \text{E}[\text{Var}(R)] = \text{Var}(X) - \text{Var}(\text{E}[X|R]) = \Sigma^* - \text{Var}(\text{E}[X|R]),
\]

where \( X \sim N(\mu^*, \Sigma^*) \). Consider the following transformation \( Z = (\Sigma^*)^{-1/2}(X - \mu^*) \). It is well known that \( Z \) has a standard normal distribution whose covariance matrix is equal to the identity matrix \( I \). Therefore, (B.10) can be further expanded to

\[
(B.10) = (\Sigma^*)^{-1}(\Sigma^* - \text{Var}(\text{E}[X|R]))(\Sigma^*)^{-1}(\mu - \mu^*) + O(\|\mu^* - \mu\|_2^2)
= (\Sigma^*)^{-1}(\Sigma^* - (\Sigma^*)^{1/2}\text{Var}(\text{E}[Z|R'])(\Sigma^*)^{1/2})(\Sigma^*)^{-1}(\mu - \mu^*) + O(\|\mu^* - \mu\|_2^2)
= (\Sigma^*)^{-1/2}(I - \text{Var}(\text{E}[Z|R']))(\Sigma^*)^{-1/2}(\mu - \mu^*) + O(\|\mu^* - \mu\|_2^2),
\]

where \( R' \) represents the transformed regions in the \( Z \)-space.

Suppose Assumption 1 holds. In this case, we know that

\[
\lambda_{\max}(I - \text{Var}(\text{E}[Z|R'])) \leq 1 - \epsilon.
\]

As a result,

\[
\| (\Sigma^*)^{-1/2}(I - \text{Var}(\text{E}[Z|R']))(\Sigma^*)^{-1/2} \|_2 \leq (1 - \epsilon)\lambda_{\max}((\Sigma^*)^{-1}) = (1 - \epsilon)\lambda_{\min}(\Sigma^*)^{-1}
\]

This implies that there exists a small neighborhood \( B_2(r; \mu^*) \), such that for \( \mu \in B_2(r; \mu^*) \), we have

\[
\| \nabla Q(M(\mu) | \mu) - \nabla Q(M(\mu) | \mu^*) \|_2 \leq \| (\Sigma^*)^{-1/2}(I - \text{Var}(\text{E}[Z|R']))(\Sigma^*)^{-1/2} \|_2 \| \mu - \mu^* \|_2 + o(\|\mu - \mu^*\|_2)
\leq (1 - \epsilon)\lambda_{\min}((\Sigma^*)^{-1})\| \mu - \mu^* \|_2 + o(\|\mu - \mu^*\|_2).
\]

For a sufficiently small \( r \), we can guarantee that (B.8) holds.

Proof. Proof of Theorem 1. The desired result is a direct implication of (Balakrishnan et al. 2017, Theorem 4), which requires Lemmas B.1 and B.2, respectively. We set \( \lambda = \frac{1}{\min(\text{eig}(\Sigma^*))} \) and \( \gamma = \frac{1 - \epsilon/2}{\min(\text{eig}(\Sigma^*))} \), where \( \gamma < \lambda \) for any \( 0 < \epsilon \leq 1 \). Therefore, using (Balakrishnan et al. 2017, Theorem 4), we have

\[
\| M(\mu) - \mu^* \|_2 \leq (1 - \epsilon/2)\|\mu - \mu^*\|_2, \quad \text{for all} \ \mu \in B_2(r; \mu^*).
\]

(B.11)

Then, we immediately derive that for any initial point \( \mu^{(0)} \in B_2(r; \mu^*) \), the population EM sequence \( \{\mu^{(t)}\}_{t=0}^{\infty} \) exhibits linear convergence, and establish the desired result.

B.3 Hierarchical Bayesian model

In this section, we first present the Metropolis Hasting algorithm to estimate the posterior distribution. Then we optimize this method and use a Bayesian grid search algorithm which performs better in terms of speed and accuracy.
Algorithm 3 Metropolis Hasting
1: Input: $R_{cn}^{(t)}$, $\mu^{(t)}$, $\Sigma^{(t)}$
2: while $error \leq \epsilon$ do
3: simulate $\mu^{(t)} = \mu^{(t)} + \epsilon$, $\Sigma^{(t)}$
4: $\epsilon \sim \text{unif}(-0.5, 0.5)$
5: Calculate $P(R_{cn}^{(t)} | \mu^{(t)}, \Sigma^{(t)}) \times P(\mu^{(t)}) \times P(\Sigma^{(t)})$
6: Calculate $P(R_{cn}^{(t)} | \mu^{(t)}, \Sigma^{(t)}) \times P(\mu^{(t)}) \times P(\sigma^{(t)})$
7: $A = \frac{P(R_{cn}^{(t)}, \mu^{(0)}, \sigma^{(0)})}{P(R_{cn}^{(t)}, \mu^{(0)}, \sigma^{(0)}) \times P(\mu^{(0)}) \times P(\sigma^{(0)})}$
8: $a \sim \text{Unif}(1)$
9: if $a \leq A$ then
10: $\mu^{(t)} = \mu^{(t+1)}$, $\Sigma^{(t)} = \Sigma^{(t+1)}$
11: else
12: $\mu^{(t)} = \mu^{(t)}$, $\Sigma^{(t)} = \Sigma^{(t)}$
13: end if
14: $error \leftarrow \|\mu^{(t+1)} - \mu^{(t)}\|_1 + \|\Sigma^{(t+1)} - \Sigma^{(t)}\|_1$, $t \leftarrow t + 1$
15: end while
16: return $\mu^{(t)}$, $\Sigma^{(t)}$

Algorithm 4 Bayesian Grid Search
1: Input: $R_{cn}^{(t)}$, prior($\mu^{(t)}$), prior($\Sigma^{(t)}$)
2: while $error \leq \epsilon$ do
3: Simulate $\mu^{(t)}$, $\Sigma^{(t)}$
4: Calculate $P(R_{cn}^{(t)} | \mu^{(t)}, \Sigma^{(t)})$
5: Calculate $P(R_{cn}^{(t)} | \mu^{(t)}, \Sigma^{(t)}) \times P(\mu^{(t)}) \times P(\Sigma^{(t)})$
6: Calculate $P(\mu^{(t)}, \Sigma^{(t)} | R_{cn}^{(t)}) \times P(\mu^{(t)}) \times P(\Sigma^{(t)})$
7: $error \leftarrow \|\mu^{(t+1)} - \mu^{(t)}\|_1 + \|\Sigma^{(t+1)} - \Sigma^{(t)}\|_1$, $t \leftarrow t + 1$
8: end while
9: search the maximum posterior return maximum posterior $\mu$ and $\Sigma$