Synthetic Data Sets with Non-Constant Substitution Patterns for Fare Class Choice

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1. Introduction

Synthetic data sets that are based on discrete choice models are applied in various research areas. A major field of study utilizing generated data focuses on the properties of newly developed discrete choice models and their predictive performance (Chiou and Walker, 2007). A prominent example is the Mixed Logit model whose development has led to an increase in studies applying synthetic data (Garrow et al., 2010). In addition to testing the performance of discrete choice models by applying synthetic data sets as done by Walker (2001, pp. 57), generated data is also applied to verify estimation results obtained by new estimators. In this context, Bierlaire et al. (2008) provide a study based on the comparison of two estimators for choice based samples. Synthetic data also provides the basis for evaluating the process of data generation itself. For instance, Garrow et al. (2010) compare three methodologies for generating such data and offer recommendations based on their empirical findings. Another option for applying generated data occurs when real data is not available. In mathematical optimization models disaggregate choice decisions from synthetic data can be utilized to represent demand for a certain product or service. For example, in revenue management in the airline industry the seat inventory control provides a solution to whether a seat in a fare class is offered to a passenger for a certain price (Andersson, 1998). Therefore, demand data is needed. In a discrete choice context this requires the generation of utility functions at the level of the decision maker, i.e. the individual. According to its respective definition, the deterministic part of utility may contain variables like travel cost, in-vehicle travel time, out- of-vehicle travel time and distance as well as income, gender and trip purpose (Williams and Ortuzar, 1982). When applying synthetic data these values are generated using probability distributions that can be verified by real data. The stochastic part of utility is then generated according to the assumptions the modeler makes about the underlying choice behavior of the generated population. Specifically in airline revenue management accurate data on fare class choice decisions is not available or is lacking important information (Hess et al., 2010).

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To fill this gap, this paper provides a methodology to generate synthetic data for this purpose. Thereby it is assumed that the provided approach is valid for the case of a single flight with fixed capacity between a certain city pair. Furthermore, the airline as a monopolist is able to differentiate the fares offered to customers on that particular flight. This construct is known as price discrimination (Talluri and Van Ryzin, 2005, pp. 352-363). For data generation we assume in the following, that the utility a passenger receives from choosing a particular fare is dependent on product attributes, individual characteristics as well as factors that are not observed by the modeler. These unobserved factors are assumed to be correlated over alternatives and to have an important impact on demand by causing non-constant substitution between these fare classes (Berry, 1994). Insights on the methodology used to generate individual discrete choice utility values with constant and non-constant substitution patterns are given in section 2 . Assumptions regarding the attributes of the considered alternatives as well as the characteristics of the generated population are provided in section 3. Furthermore, estimation results and elasticities are presented proving that the assumed substitution patterns are well recovered by the generated data.

2. Modeling Framework

Our considerations regarding the demand model for fare class choice are based on the theoretical framework of random utility theory. According to Marschak (1960) a choice model derived under the assumption that a decision maker maximizes its personal utility is called a random utility model (RUM). Thereby, utility is a random variable from the researcher's perspective as some influences affecting the choice decision usually remain unknown. Discrete choice models belong to this category of models (McFadden, 1974).

In this context, we consider fare class choice in airline revenue management. Airline passengers indexed $n = 1, \dots, N$ are assumed to choose exactly one fare class f out of an individual choice set C_n. The number of choice alternatives in C_n is required to be finite and exhaustive. Furthermore, alternatives within the choice set are mutually exclusive (Train, 2009, p. 15).

2.1. Utility and Decision Rule

Passengers are assumed to evaluate each fare class according to fare class attributes. Choices are further influenced by passenger characteristics. Each passenger n receives a certain utility u_{nf} of choosing fare class f. Utility u_{nf} is decomposed into a deterministic part v_{nf} and a stochastic part ε_{nf} and is formally defined as

$$u_{nf} = v_{nf} + \varepsilon_{nf} \tag{2.1}$$

with

$$v_{nf} = \sum_{k} \beta_{fk} z_{nfk} \,. \tag{2.2}$$

Pursuant to random utility theory a decision maker chooses the alternative with highest utility. Hence, the decision rule for the fare class choice problem can be stated as follows: A passenger n chooses fare class f only if $u_{nf} > u_{nf'} \forall f \neq f'$ (McFadden, 2001; Ben-Akiva and Lerman, 1985, p. 101). The probability of choosing fare class $f \in C_n$ over fare class f' is then defined by

$$\begin{aligned} P_{nf} &= Prob\ (u_{nf} \geq u_{nf'}, \forall f' \in C_n, f' \neq f) \\ &= Prob\ (v_{nf} + \varepsilon_{nf} \geq v_{nf'} + \varepsilon_{nf'}, \forall f' \in C_n,\ f' \neq f) \\ &= Prob\ (\varepsilon_{nf'} \leq v_{nf} - v_{nf'} + \varepsilon_{nf}, \forall f' \in C_n,\ f' \neq f) \end{aligned} \tag{2.3}$$

Given a specific assumption about the joint distribution of the stochastic utility component any choice model can be derived from equation 2.3 (Ben-Akiva and Lerman, 1985, p. 101). Thus, the specification of the joint distribution of ε_{nf} differs according to the choice model the researcher believes best represents the underlying choice situation.

2.2. Generation of Stochastic Utility

In a synthetic data set the stochastic utility component is generated such that the assumed behavioral process can be represented by the choice model that is considered for the data generation process. In simulation this approach is known as input modeling. Hence, to generate data that complies with our assumptions regarding the behavioral process for fare class choice we consider probability distributions according to a Multinomial Logit (MNL) and Nested Logit (NL) model for the generation of ε_{nf}. The disturbances of the discrete choice utilities are simulated by applying a pseudo random number generator (Garrow et al., 2010; Rosenthal, 2004).

An alternative approach to generate synthetic discrete choice data sets includes the utilization of NL choice probabilities to determine chosen alternatives. According to Garrow et al. (2010) the approximation of Gumbel distributed random variables with normals should be avoided as it yields biased data sets that do not reflect the desired behavioral model.

2.2.1 MNL Errors

The MNL model is derived from equation 2.3 if we assume that ε_{nf} is independently and identically (iid) type I[1] extreme value (EV) distributed with location parameter η and scale parameter μ (Train, 2009, p. 38). Thus, MNL error terms are distributed with density

$$f\left(\varepsilon_{nf}\right) = \mu e^{-\mu(\varepsilon_{nf}-\eta)} e^{e^{-\mu(\varepsilon_{nf}-\eta)}} \tag{2.4}$$

[1] The type I extreme value distribution is also referred to as Gumbel distribution (Coles et al., 2001, pp. 46-48).

and cumulative distribution

$$F(\varepsilon_{nf}) = e^{-e^{-\mu(\varepsilon_{nf}-\eta)}}. \tag{2.5}$$

Let $F(\varepsilon_{nf}) = d$ be the probability of retrieving a draw that is equal or below ε_{nf} with d being a number between zero and one. Then, we can define $F(\varepsilon_{nf}) = \delta$ with δ being a draw of the standard uniform distribution. By solving for ε_{nf} we obtain a draw from distribution 2.5 as $\varepsilon_{nf} = F^{-1}(\delta) = \frac{1}{\mu}(-\ln(-\ln(\delta))) + \eta$ for decision maker n and a fare class f (Train, 2009, pp. 209-210). The inverse cumulative distribution of equation 2.5 is denoted by $F^{-1}(\delta)$ and is also called the quantile function $Q(\delta)$ (Gilchrist, 2000, pp. 12-14). The cumulative distribution function (CDF) $F(\cdot)$ is always invertible in a unique way if the argument is univariate and the corresponding probability density is nonzero.

The value of μ in the MNL model is arbitrary as it only sets the scale of the utilities. Thus, for convenience μ is usually chosen to equal one (Ben-Akiva and Lerman, 1985, p. 71). Without loss of generality, the location parameter is assumed to be $\eta = 0$ if a full set of alternative-specific constants (i.e., $|C| - 1$ constants in the considered fare class choice problem with $C = \bigcup_n C_n$) is included in the choice model (Hunt, 2000).

2.2.2 Substitution Patterns

By definition, the MNL model is not able to capture correlations between alternatives as the unobserved utility components for different alternatives are unrelated (Train, 2009, p. 39). Fare classes on a single flight are defined as differing products exhibiting several combinations of travel restrictions as well as differing prices. They are distinguished by compartment (first, business and economy) and are further characterized by additional benefits customers gain beyond the actual flight between an origin and destination. Within each of the mentioned compartments fare classes exhibit similar characteristics like advance purchase requirements, length-of-stay requirements, rebooking and cancellation penalties, the possibility to upgrade, the possibility to collect frequent flyer miles and many more. More complex combinations of restrictions imposed on a fare class result in lower prices (Talluri and Van Ryzin, 2005, pp. 521). Restrictions, thus, provide a necessary fencing between low and high fare products to prevent certain customers (i.e., business travelers) from buying down to a cheaper fare class (Zhang and Bell, 2010).

A buy down occurs when a customer who is willing to purchase a high fare product in the first place actually chooses a discount fare when both products are available. Thus, fencing serves as a justification for the disregard of up sell and down sell between fare classes. In particular, high fare customers are discouraged from purchasing low fare tickets as fare restrictions reduce the attractiveness of cheaper fares (Fiig et al., 2010).

As various fares on a single flight provide customers with similar restrictions we suppose that dependencies in demand between alternatives with common characteristics exist. Hence, MNL substitution patterns that are constant between alternatives represent an inappropriate assumption for the considered fare class choice problem.

However, in airline revenue management research it is common practice to assume that demand for alternatives offered at the same time is independent. This is also known as the independent demand assumption. Thereby, demand for each fare class is supposed to be an independent stochastic process that is not influenced by the availability of other alternatives. An endogenization of customer behavior is not considered in the independent demand model (Talluri and Van Ryzin, 2005, p. 301).

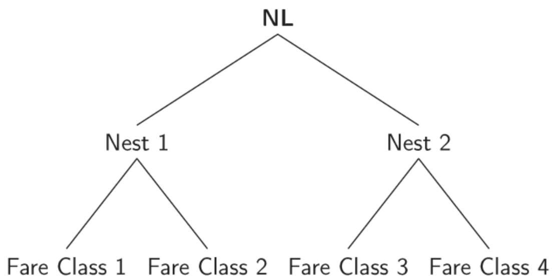
We presume, in the following, that correlation between fare classes is caused by the above mentioned fare attributes that are not included in the deterministic utility component v_{nf}. According to Berry (1994) these unobserved factors have important influence on demand as they lead to non-constant substitution patterns.

To account for the supposed demand dependencies between available alternatives our approach focuses on the generation of synthetic data based on a discrete choice model with more flexible substitution patterns. The NL model, for instance, is able to account for correlation in unobserved factors of alternatives and provides a more realistic representation of choice behavior.

2.2.3 NL Errors

Individual choices that comply with an NL model can be derived by assuming that the stochastic utility components of equation 2.3 follow a generalized extreme value (GEV) distribution (Train, 2009, pp. 80-81). For further details on the derivation of the NL choice probabilities see McFadden et al. (1978).

Figure 1 – NL nesting structure for a two-level NL model with four alternatives grouped into two nests.



Source: Own illustration

The assumption stated above, allows the grouping of alternatives that share common unobserved attributes into $m = 1, \dots M$ non-overlapping nests. Thus, the stochastic utility component ε_{nf} of equation 2.1 can be decomposed into a nest specific term ε_{nm} that is the same for all alternatives in nest m and an alternative specific term ε_{nfm} that is independent across all alternatives (Bhat, 1996). The sum of both disturbances again has the same variance as the disturbance of the MNL model (Ben-Akiva and Lerman, 1985, p. 287). A general example on the nesting of four alternatives in a two-level NL model is given in figure 1. Although, the choice decision according to an NL model is not a hierarchical process we distinguish between the upper (nest) level and lower (alternative) level choice decision to derive the required terms for the data generation procedure.

Individual utility for choosing an alternative according to the NL model is obtained as

$$u_{nf} = v_{nf} + \varepsilon_{nm} + \varepsilon_{nfm} \quad \forall\, n, f \in C_{nm}|m \qquad (2.6)$$

where C_{nm} denotes the choice set of individual n for a given nest m. The error terms ε_{nfm} are iid Gumbel distributed with scale parameter μ_m whereas the distribution of ε_{nm} is not known (Garrow et al., 2010). The ε_{nfm} are generated according to the procedure for the MNL error terms as stated in section 2.2.1. The scale parameter μ_m hereby describes the variances of the unobserved effects of utility u_{nf} on the lower level of the nesting structure. Thus, for all alternatives in the same nest m the scale parameter μ_m is identical. Alongside the decomposition of the total error term ε_{nf} in equation 2.6 we also consider a compound error term for the generation of stochastic utility in the NL model as

$$\bar{\varepsilon}_{nf} = \varepsilon_{nm} + \tilde{\varepsilon}_{nfm} \; \forall \; n, f \in C_{nm}|m \tag{2.7}$$

Thereby, ε_{nm} is the disturbance associated with the choice decision of an individual n on the upper level of the choice problem while $\tilde{\varepsilon}_{nfm}$ is the disturbance of the maxima of the individual utilities associated with the lower level choice decision. For each individual, the choice decision on the lower level is determined by the maximum of the utility values associated with the available alternatives. In the following, this maximum is denoted by $\tilde{u}_{nf}$.

The compound error $\bar{\varepsilon}_{nf}$ from equation 2.7 is non-independently and identically Gumbel distributed with scale parameter μ (Hunt, 2000; Silberhorn et al., 2008).

In an NL model formulation only the ratio of the two scale parameters μ/μ_m can be identified from the data. Therefore, the scale of utility is set by normalizing one of the scale parameters to one. The decision as to which parameter is to normalize is arbitrary as either possibility results in the same model (Ben-Akiva and Lerman, 1985, p. 287; Hensher and Greene, 2002). For the sake of generalization we will in the following illustrate the generation of the NL error terms by explicitly considering both scale parameters within the formal representations. Thus, the data generation process can be easily reproduced regardless of the normalization applied by the modeler.

The difficulty in generating a data set with the desired NL correlation structure lies in the disturbances ε_{nm} that are distributed such that the maxima of the individual utility values, $\tilde{u}_{nf}$, are iid Gumbel distributed with scale parameter μ. This is an indirect conclusion as the distribution of ε_{nm} is unknown. However, it can be obtained from the information about the mean value and variance of the compound error $\bar{\varepsilon}_{nf}$ and the independent errors of each individuals maximum utility $\tilde{\varepsilon}_{nfm}$ (Garrow et al., 2010). Therefore, in the following we utilize the relation of these error terms as given by equation 2.7.

In general, the mean value and variance of an iid type I EV random variable X with location parameter η and scale μ are formally given by

$$E(X) = \eta + \frac{\gamma}{\mu} \tag{2.8}$$

and

$$Var(X) = \frac{\pi^2}{6\mu^2} \tag{2.9}$$

with γ being Euler's constant.

According to Ben-Akiva and Lerman (1985, pp. 104-105) the maximum of $|C|$ iid Gumbel distributed random variables (i.e.; $\tilde{\varepsilon}_{nfm}$) with location and scale parameters $(\eta_1, \mu_m), (\eta_2, \mu_m), \ldots, (\eta_F, \mu_m)$ is also iid Gumbel distributed with parameters

$$\left(\frac{1}{\mu_m} \ln \sum_{f \in C_{nm}} e^{\mu_m \eta_f}, \mu_m \right). \tag{2.10}$$

Furthermore, the variance of the independent error term is

$$Var(\varepsilon_{nfm}) = \frac{\pi^2}{6\mu_m^2} \tag{2.11}$$

and since $\eta_f = 0$, together with 2.8 and 2.11, its mean value is

$$E(\varepsilon_{nfm}) = \frac{\gamma}{\mu_m}. \tag{2.12}$$

Following Hunt (2000) the location parameter of an iid Gumbel distributed random variable can be set to zero, as any nonzero location parameter is eliminated by an alternative-specific constant. Assuming a full set of constants in our choice model we can set $\eta_f = 0$. Hence, the location parameter of the distribution of the maximum values of the independent disturbances $\tilde{\varepsilon}_{nfm}$, becomes

$$\tilde{\eta} = \frac{1}{\mu_m} \ln |C_{nm}|. \tag{2.13}$$

Substituting 2.13 in 2.8, we derive the mean value of the disturbance maxima as

$$E(\tilde{\varepsilon}_{nfm}) = \frac{1}{\mu_m} \ln |C_{nm}| + \frac{\gamma}{\mu_m}. \tag{2.14}$$

Furthermore, the variance of $\tilde{\varepsilon}_{nfm}$ equals the variance of ε_{nfm}:

$$Var(\tilde{\varepsilon}_{nfm}) = \frac{\pi^2}{6\mu_m^2}. \tag{2.15}$$

To derive the unknown distribution of ε_{nm} we need the mean value and the variance of the compound error from equation 2.7. Both values are defined as

$$E(\bar{\varepsilon}_{nfm}) = E(\varepsilon_{nm} + \tilde{\varepsilon}_{nfm}) = \frac{\gamma}{\mu} \tag{2.16}$$

and

$$Var(\bar{\varepsilon}_{nfm}) = Var(\varepsilon_{nm} + \tilde{\varepsilon}_{nfm}) = \frac{\pi^2}{6\mu^2}. \tag{2.17}$$

Having made the above definitions the derivation of the mean value and variance of ε_{nm} is now straightforward. From equations 2.14, 2.16, 2.15 and 2.17 we obtain the mean value and variance of ε_{nm} as

$$\begin{aligned} E(\varepsilon_{nm}) &= E(\bar{\varepsilon}_{nfm}) - E(\tilde{\varepsilon}_{nfm}) \\ &= \left(\frac{1}{\mu_m}\ln\ |C_{nm}|\right) + \left(\frac{\gamma}{\frac{\mu_m\mu}{\mu_m-\mu}}\right) \end{aligned} \tag{2.18}$$

and

$$\begin{aligned} Var(\varepsilon_{nm}) &= Var(\bar{\varepsilon}_{nfm}) - Var(\tilde{\varepsilon}_{nfm}) - 2Cov(\varepsilon_{nm}\ \tilde{\varepsilon}_{nfm}) \\ &= \frac{\pi^2}{6\mu^2} - \frac{\pi^2}{6\mu_m^2} - 0 \\ &= \frac{\pi^2}{6\left(\frac{\mu_m^2\mu^2}{\mu_m^2-\mu^2}\right)}\ . \end{aligned} \tag{2.19}$$

As mentioned before, the independent error term ε_{nfm} from the NL utility function 2.6 is Gumbel distributed with location parameter 0 and scale parameters μ_m. As the scale parameters μ_m are predetermined by the modeler the disturbance is obtained according to the generation of the MNL errors as described in section 2.2.1. From equations 2.18 and 2.19 we get the location and scale parameter of the nest specific error terms ε_{nm}:

$$\left[\underbrace{-\left(\frac{1}{\mu_m}\ln\ |C_{nm}|\right)}_{location\ parameter};\ \underbrace{\sqrt{\left(\frac{\mu_m^2\mu^2}{\mu_m^2-\mu^2}\right)}}_{scale\ parameter}\right]. \tag{2.20}$$

The NL disturbances can now be generated by combining the inverse of the Gumbel cumulative distribution function with the parameters from 2.20:

$$\varepsilon_{nm} = F^{-1}(\delta) = \frac{1}{\mu}\left(-\ln(-\ln(\delta))\right) + \eta$$

$$= \frac{1}{\left(\frac{\mu_m^2\mu^2}{\mu_m^2-\mu^2}\right)}\left(-\ln(-\ln(\delta))\right) - \left(\frac{1}{\mu_m}\ln\ \ |C_{nm}|\right) \tag{2.21}$$

with δ being a uniform [0, 1] distributed random variable.

2.2. Generation of Systematic Utility

For the generation of the deterministic part of utility v_{nf}, we consider $k = 1,\dots,3$ observable attributes of the alternatives as well passenger characteristics. According to equation 2.2 coefficients β_{fk} provide a weighting regarding the influence of each observed factor z_{nfk} on deterministic utility v_{nf}. Let

$$v_{nf} = \beta_{f0} + \beta_1 \cdot z_{nf1} + \beta_{f2} \cdot z_{n2} + \beta_{f3} \cdot z_{n3} \qquad \forall\, n, f \tag{2.22}$$

be the function of the deterministic part of individual utility for the fare class choice problem.

2.3.1 Attributes and Characteristics z_{nfk}

According to equation 2.22 the value of v_{nf} depends on

- the price payed by passenger n for a ticket in fare class f - z_{nf1},
- passengers gender - z_{n2} and
- the trip purpose of passenger n - z_{n3}.

As for the error terms, values for these variables are again generated by making assumptions about their distribution across the synthetic population. Characteristics gender and trip purpose, are dummy variables and can easily be generated by drawing from a uniform [0,1] distribution. Prices for each passenger and fare class are assumed to be truncated normally distributed random variables.

2.3.2 Coefficients β_{fk}

Each of the considered attributes z_{nfk} is weighted by a coefficient β_{fk}. For existing real data on a specific choice problem these coefficients are determined by estimation. Hence, in a data generation context these coefficients are chosen to ensure that the data set reflects the assumptions regarding the influence of each attribute and characteristic on individual utility. Furthermore, it is important that neither the deterministic part nor the stochastic part of utility dominates the overall utility value u_{nf} (Munizaga et al., 2002). Therefore, the values of the two utility components of equation 2.1 and their respective influence on the overall value of utility u_{nf} have to be verified and adjusted prior to data generation.

Further details on the specification of the values of the variables z_{nfk} and the coefficients β_{fk} are provided in section 3.

3. Fare Class Choice

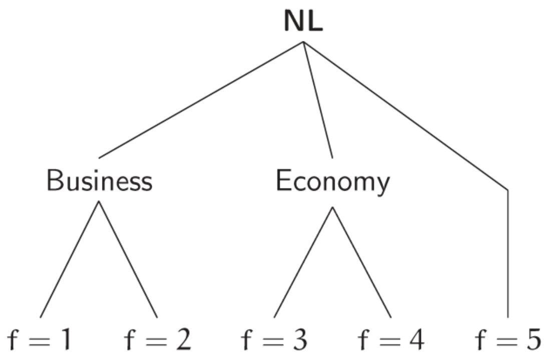
Since the liberalization of the airline market in the early 1970s airlines have started to utilize price discrimination for differentiated products as an instrument to maximize revenues (McGill and Van Ryzin, 1999; Anderson et al., 1992, pp. 1-5). Based on this, we suppose that the considered fare class choice problem is described by the choice decision between four ticket fares and a no choice option. We act on the assumption that the following alternatives exist:

- a regular ($f = 1$) and a discount fare ($f = 2$) in business class,
- a regular ($f = 3$) and a discount fare ($f = 4$) in economy class, and
- a no choice option ($f = 5$).

The no choice option expresses the decision of a potential customer to not buy a ticket in a certain fare class at all. It further ensures that the choice set of each generated individual is realistic and exhaustive. In the presented approach the alternative $f = 5$ serves as the reference alternative of the choice model. Furthermore, it is not assigned an attribute value for fare class price as the decision of not choosing an alternative is assumed to not impose any cost on a particular passenger. The functions of deterministic utility for a passenger n are defined as follows:

$$V_{n1} = \beta_{10} + \beta_1 \cdot z_{n11} + \beta_{12} \cdot z_{n2} + \beta_{13} \cdot z_{n3}$$
$$V_{n2} = \beta_{20} + \beta_1 \cdot z_{n21} + \beta_{22} \cdot z_{n2} + \beta_{23} \cdot z_{n3}$$
$$V_{n3} = \beta_{30} + \beta_1 \cdot z_{n31} + \beta_{32} \cdot z_{n2} + \beta_{33} \cdot z_{n3}$$
$$V_{n4} = \beta_{40} + \beta_1 \cdot z_{n41} + \beta_{42} \cdot z_{n2} + \beta_{43} \cdot z_{n3}$$
$$V_{n5} = 0$$

Figure 1 - Assumed nest structure for utility generation in a fare class choice demand model.



Source: Own illustration

As already stated in the previous section fare class attributes for the remaining alternatives as well as passenger characteristics have to be defined.

Thereby, prices z_{nf1} in € for each passenger n and fare class f are assumed to be normally distributed $N(\mu, \sigma)$ random variables with mean μ and standard deviation σ:

- $\mu = 1000, \sigma = 200$ for f=1,
- $\mu = 800, \sigma = 150$ for f=2,
- $\mu = 400, \sigma = 100$ for f=3,
- $\mu = 200, \sigma = 50$ for f=4.

The data set is furthermore generated such that 47% of the passengers of the synthetic population are female and 53% male, respectively. Additionally, the population can be segmented in passengers traveling for leisure or business purposes. Thereby, passengers with leisure trips represent 72% of the population and passengers with business trips the remaining 28% (Brey and Walker, 2011).

As for the coefficients β_{fk}, we have to make sure that the assumptions made about the influence of the attributes and characteristics on the deterministic utility of each alternative are reflected by the synthetic data. The corresponding coefficient values that are applied in the data generation process are displayed in column '*true value'* in table 1.

Besides true coefficient values the estimates for both an NL model and an MNL model are compared. Estimates are obtained from the synthetic data set with NL errors.

By setting the true coefficient values, we first assume that the alternative specific constants (ASC) β_{f0} provide the desired market shares of the fare classes considered in our choice model. Second, price sensitivity is included in the behavioral model by assuming that a higher price decreases the utility value an individual receives from choosing a certain fare class. This is achieved by assuming a negative price coefficient β_1 that is the same for all alternatives. This is known as generic specification (Garrow et al., 2007).

Table 1 - True and estimated coefficients of the synthetic data set with confidence levels ***= 99%, ** = 95% and * = 90%.

Coefficient		NL			MNL		
β_{fk}	True value	Estimate	t-statistic against zero	t- statistic against true value	Estimate	t-statistic against zero	t- statistic against true value
ASC							
β_{10}	0.50	0.065	0.27	-1.81*	0.348	1.33	-0.58
β_{20}	1.50	1.560	8.34***	0.32	2.310	16.14***	5.66***
β_{30}	1.60	1.420	20.08***	- 2.24***	1.160	13.77***	-5.24***
β_{40}	2.00	1.820	31.66***	-3.14***	1.980	38.54***	-0.39
β_{50}	0.00	0.00	-	-	-	-	-
Price							
β_1	-0.0040	-0.00427	-17.55***	-1.11	-0.00535	-30.78***	-7.76***
Gender							
β_{12}	0.80	0.899	5.47***	0.60	0.930	4.58***	0.64
β_{22}	0.50	0.561	6.51***	0.71	0.537	6.47***	0.42
β_{32}	0.20	0.184	3.01***	-0.26	0.299	4.27***	1.41
β_{42}	-0.10	-0.0934	-1.83*	0.13	-0.124	-2.40***	-0.46
β_{52}	0.00	0.00	-	-	-	-	-
Trip Purpose							
β_{13}	2.00	2.290	12.53***	1.58	2.560	12.18***	2.67***
β_{23}	1.50	1.380	14.84***	-1.29	1.360	14.26***	-1.47
β_{33}	1.00	1.070	14.15***	0.93	1.280	16.08***	3.53***
β_{43}	0.50	0.557	8.60***	0.88	0.496	7.56***	-0.06
β_{53}	0.00	0.00	-	-	-	-	-
Nest Coefficients[2] μ_m							
μ_1	1.80	1.40	8.75***	-2.50***			
μ_2	1.60	1.570	13.76***	-0.26			
μ_3	1.00	1.00	-	-			

[2] The value of the t-statistic as displayed for the nest coefficients tests the null hypothesis that $\mu_m = 1$ for all m.

Source: Own calculations

Finally, coefficients β_{f2} and β_{f3} provide a weighting of the socio-economic characteristics gender and trip purpose that are both included in the choice model as dummy variables. As both characteristics do not vary across alternatives the corresponding coefficients are defined alternative-specific. We further assume male business ($z_{nf2} = 1$, $z_{nf3} = 1$) travelers to receive higher utility from choosing a business fare over economy. Buying a ticket in business class is, due to better seat comfort and less restrictive regulations regarding rebooking and cancellation, supposed to have a positive effect on utility for male passengers as well as business travelers.

The latter are generally considered relatively price-insensitive (Talluri and Van Ryzin, 2005, pp. 516-517) while leisure travelers, in particular, are found to have a higher price-sensitivity than business travelers (Garrow, 2010, pp. 18-19).

In equation 2.22 that represents the functional form of utility for our fare class choice problem, we do not account for fare flexibility, amenities like lounge access, seating on board or preferences of customers associated with business or economy class within the specification of v_{nf}. However, these attributes have an important influence on the utility value an individual receives from choosing a particular alternative as well as on substitution patterns between alternatives.

As outlined in section 2.2.3 we assume that these unobserved effects are completely captured by ε_{nf} leading to correlation in alternatives with similar restrictions.

Hence, the alternatives of the considered fare class choice problem are assigned to $m = 1,\dots,3$ nests in the following way:

- Nest 1: $f = \{1,2\}$
- Nest 2: $f = \{3,4\}$
- Nest3: $f = \{5\}$.

The corresponding nesting structure is displayed in figure 2. It reflects the assumption that business fares and economy fares are closer substitutes among each other than are fares from other nests. Substitution patterns in the NL model are by definition constant between fare classes in the same nest but not constant across nests. Hence, the independence of irrelevant alternatives (IIA) assumption holds within each nest but not in general for alternatives that are assigned to different nests (Train, 2009, p.81). This is justified by the fact that more price sensitive leisure passengers book their trips way in advance and tend to choose the least expensive option. On the contrary, business travelers are known to choose fares that allow for additional amenities at the airport and on board. As business travelers tend to be more time sensitive they also prefer the possibility to cancel or rebook a flight on a short notice if appointments change (Garrow et al., 2007).

To achieve the desired correlation structure for our fare class choice problem, the nest coefficients μ_m for $m = 1,\dots,3$ are provided for the generation of the NL error term. These coefficients allow for alternatives within the same nest to be closer substitutes than alternatives from different nests resulting in flexible substitution patterns. They are the same for all alternatives in one nest. As alternative $f = 5$ is solely assigned to the third nest, leading to a degenerate nesting structure, we choose $\mu_3 = 1$ for identification purposes.

3.1. Data Sets

As proposed by Garrow et al. (2010) a synthetic data set with 10.000 observations and correlation structure as proposed in the previous section is generated. Both an NL model and an MNL model are estimated from the data. We hereby assume that the behavioral process according to an NL model represents the true choice behavior of airline passengers. Estimates as displayed in table 1 are obtained by estimation with BIOGEME version 2.2 (Bierlaire, 2003). Besides true and estimated coefficients β_{fk} for both the NL and MNL models, the corresponding t-statistics against zero and significance levels are provided. Except for the NL and MNL estimate of the alternative-specific constant β_{10} the null hypothesis is rejected at the 99% level of confidence for the remaining estimates.

Regarding the nest coefficients the null hypothesis of the t-statistic is $\mu_m = 1$ for all nests m confirming that the nest coefficients are statistically significant on a 99% level of confidence.

Column *'t-statistic against true value'* displays the value of the t-statistic for each estimate and nest coefficient against its corresponding true coefficient value. Results show that the true coefficients provided for data generation are well recovered for the NL model. However, we have to reject the null hypothesis that NL estimates β_{30} and β_{40} as well as nest coefficient μ_1 equal their respective true value on a 99 % level of confidence. Although, we cannot be sure whether the estimated coefficients are equal to the true coefficients we can confirm, by the corresponding t-tests against zero, that all three estimates have significant influence on the individual utility values.

As the MNL estimates are obtained from a data set with an NL error structure the value of the t-statistic against the true coefficient value in the MNL yields that the null hypothesis has to be rejected for β_{20}, β_{30}, β_1, β_{13} and β_{33} on a 99% level of confidence.

Nest coefficients μ_1, μ_2 and μ_3 are only obtained for the NL model and reflect the degree of correlation between alternatives within the same nest. Correlation for any pair of alternatives in a common nest can be determined by calculating $\kappa_m = 1 - \left(\frac{\mu}{\mu_m}\right)$ with $m = \{1,2,3\}$. Thereby, as proposed in section 2.2, μ is the upper level scale parameter of the NL model and is set to one for identification purposes (Ben-Akiva and Lerman, 1985, p. 287). The correlation matrix associated with our fare class choice problem is

$$\begin{pmatrix} 1 & \kappa_1 & 0 & 0 & 0 \\ \kappa_1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \kappa_2 & 0 \\ 0 & 0 & \kappa_2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.1}$$

with $\kappa_1 = 0.49$ and $\kappa_2 = 0.59$ being the correlation coefficients of nest 1 and nest 2, respectively. As $\mu_3 = 1$ we obtain $\kappa_3 = 0$.

3.2. Market Shares

According to the definition of the error terms in section 2.2 we assume demand shifts to be proportional in the MNL model and non-proportional in the NL model between alternatives in different nests, if a fare class is closed. The following analysis of substitution patterns is based on an exemplary comparison of each alternatives' market shares (MS) when

(i) all alternatives are available
(ii) the cheapest fare class is closed.

In airline revenue management optimization models similar decisions are part of the seat inventory control aiming on revenue maximization.

Table 2 - MNL market shares in % for situations (i) and (ii).

Fare Class	1	2	3	4	5
Market Share (i)	1.25	7.59	14.60	55.37	21.19
Market Share (ii)	2.54	16.02	31.44	-	50.00

Source: Own calculations

For the simulation of market shares for both situations we apply BIOSIM (Bierlaire, 2003). The market shares corresponding to the MNL estimates of the NL data set for the above defined situations are displayed in table 2. Clearly, the most chosen option in situation (i) is the inflexible economy tariff (alternative 4) and, as expected, the most expensive business fare (alternative 1) is the least chosen option. Now we compare our findings with situation (ii) where only four alternatives remain in the choice set of the individuals. We assume that due to a decision based on a revenue management model fare class four is closed. Thus, ca. 55% of the generated individuals are not able to purchase their first choice and switch to other available alternatives. In table 2 we see that all alternatives gain from the closure of fare class four. The initial market shares of all remaining fare classes increase by approximately 100% in situation (ii). Furthermore, we are able to observe whether the occurring demand shifts from the closed option towards the remaining alternatives are constant by calculating the ratio of substitution for any pair of alternatives. The substitution ratio for two alternatives is then obtained by dividing the respective market shares. According to the IIA assumption of the MNL we expect substitution patterns to be constant for situations (i) and (ii) (Train, 2009, pp. 49-51). Using the example of alternatives one, two and three we obtain the following substitution ratios (SR) for situations (i) and (ii):

$$SR_{13}^{MNL}(i) = \frac{MS_{f=1}}{MS_{f=3}} = \frac{1.25}{14.60} = 0.08$$

$$SR_{13}^{MNL}(ii) = \frac{MS_{f=1}}{MS_{f=3}} = \frac{2.54}{31.44} = 0.08$$
$$SR_{23}^{MNL}(i) = \frac{MS_{f=2}}{MS_{f=3}} = \frac{7.59}{14.60} = 0.51$$
$$SR_{23}^{MNL}(ii) = \frac{MS_{f=2}}{MS_{f=3}} = \frac{16.02}{31.44} = 0.51$$

As expected, substitution patterns are constant if passenger choice behavior is assumed to be best represented by an MNL model. Thus, substitution ratios between all remaining fare classes do not change if a fare class is closed for purchase. This is exemplarily presented here by comparing $SR_{13}^{MNL}(i)$ with $SR_{13}^{MNL}(ii)$ and $SR_{23}^{MNL}(i)$ and $SR_{23}^{MNL}(ii)$. Of course, the same applies for the remaining ratios. However, if we assume that some fare classes share common unobserved attributes this approach does not seem to be correct.

Table 3 - NL market shares in % for situations (i) and (ii).

Fare Class	1	2	3	4	5
Market Share (i)	1.25	7.59	14.5	55.40	21.19
Market Share (ii)	2.54	13.53	43.53	-	40.81

Source: Own calculations

Hence, in the following we examine the case where individual choice behavior is assumed to follow an NL model. For that matter, the market shares are given in table 3. According to the assumptions made above we consider the nesting structure displayed in figure 2. Note, that the displayed NL market shares for situation (i) equal the MNL market shares for situation (i). These values reflect the true market shares of the generated data set as a full set of alternative-specific constants is considered both for data generation and estimation. After closing fare class four we examine demand shifts in the NL model by exemplarily calculating the ratios of substitution for alternatives one, two and three. Thereby, alternatives one and two are members of the same nest, while alternative three belongs to a different nest. By definition, substitution patterns are constant within nests and non-constant across nests. We obtain the following results:

$$SR_{12}^{NL}(i) = \frac{MS_{f=1}}{MS_{f=2}} = \frac{1.25}{7.59} = 0.16$$
$$SR_{12}^{NL}(ii) = \frac{MS_{f=1}}{MS_{f=2}} = \frac{2.12}{13.53} = 0.16$$
$$SR_{13}^{NL}(i) = \frac{MS_{f=1}}{MS_{f=3}} = \frac{1.25}{14.57} = 0.086$$
$$SR_{13}^{NL}(ii) = \frac{MS_{f=1}}{MS_{f=3}} = \frac{2.12}{43.53} = 0.048 .$$

Clearly, substitution patterns in the NL model are as expected constant between alternatives one and two (SR_{12}^{NL}) that share a common nest. However, substitution patterns are not constant between alternatives one and three (SR_{13}^{NL}) that belong to different nests.

3.3. Elasticities

Besides market shares elasticities can also be obtained for the synthetic data sets. Elasticities represent the responsiveness of passengers to a change in a certain attribute. As in microeconomic consumer theory the price for a ticket in fare class f is the only attribute of the alternatives in the fare class choice problem. Hence, the following explanations refer to the responsiveness of the passengers of both populations regarding a change in ticket price. Therefore, the only relevant elasticity is the price elasticity. Furthermore, rather than examining disaggregate price elasticities we focus on the corresponding aggregate values (Ben-Akiva and Lerman, 1985, pp. 111-113). Elasticities are calculated based on the true coefficient values provided for data generation. Furthermore, substitution patterns according to the respective choice model are applied to obtain the responsiveness for both the NL and MNL model. The disaggregate direct and cross price elasticities for the MNL model are given by

$$\varepsilon_{z_{nfk}}^{P_{nf}} = \left[1 - P_{nf}\right] z_{nfk} \beta_k \tag{3.2}$$

and

$$\varepsilon_{z_{nf'k}}^{P_{nf}} = -P_{nf'} z_{nf'k} \beta_k . \qquad \forall\, f \neq f' \tag{3.3}$$

The values obtained by equations 3.2 and 3.3 refer to the responsiveness of an individual. In contrast, aggregate elasticities provide the responsiveness of some group of decision makers. They are the weighted averages of the individual level elasticities with weighting provided by the choice probabilities. Following Ben-Akiva and Lerman (1985, p. 113) the expected share of a group of decision makers is defined as

$$\bar{P}_{nf} = \frac{\sum_{n=1}^{N} P_{nf}}{N} \tag{3.4}$$

with N being the total number of decision makers within the respective group. Aggregate direct and cross elasticities for the MNL model are obrained by

$$\varepsilon_{z_{nfk}}^{\bar{P}_{nf}} = \frac{\sum_{n=1}^{N} P_{nf}\, \varepsilon_{z_{nfk}}^{P_{nf}}}{\sum_{n=1}^{N} P_{nf}} \tag{3.5}$$

and

$$\varepsilon_{z_{nf'k}}^{\bar{P}_{nf}} = \frac{\sum_{n=1}^{N} P_{nf}\, \varepsilon_{z_{nf'k}}^{P_{nf}}}{\sum_{n=1}^{N} P_{nf}} \tag{3.6}$$

Disaggregate and aggregate elasticities for the NL model are obtained in a similar way. For further information on the calculation of NL elasticities we refer to Koppelman and Bhat (2006, pp. 163-165).

Table 4 - NL and MNL aggregate direct price elasticities

Fare Class	1	2	3	4
NL	-2.348	-2.433	-0.743	-0.265
MNL	-3.234	-2.621	-1.129	-0.359

Source: Own calculations

Aggregate elasticities, as considered in the following, refer to the generated population as a whole. Table 4 shows the aggregate direct elasticities for both the MNL and NL model. Price sensitivity clearly seems to be less distinct in the NL model. We suspect this to be a result of the differing definition of stochastic utility as deterministic utility is identical for both models according equation 2.22. Furthermore, price changes in business class fares, as assumed, have a much higher influence on choice probabilities than price changes in economy fares. This conclusion holds for both the MNL and the NL model.

Table 5 - MNL aggregate cross price elasticities.

Fare Class	1	2	3	4
1		0.257	0.373	0.388
2	0.092		0.353	0.399
3	0.074	0.198		0.408
4	0.062	0.179	0.325	
5	0.056	0.170	0.324	0.438

Source: Own calculations

Aggregate values of the cross price elasticities are also obtained. Cross price elasticities reflect the influence on the choice probability of an alternative when the price attribute of another alternative is changed. Thereby, disaggregate cross elasticities of the MNL are uniform, i.e. equal for all alternatives $f \neq f'$ that are affected by the attribute change of alternative f (Ben-Akiva and Lerman, 1985, pp.111-113).

Tables 5 and 6 display aggregate cross price elasticities that are attained for changes in the price of one fare class and the corresponding impact on the choice probabilities of all other fare classes.

Table 6 - NL aggregate cross price elasticities.

Nest	Fare Class	1	2	3	4
1	1		1.211	0.282	0.406
1	2	0.0273		0.248	0.423
2	3	0.061	0.233		0.762
2	4	0.044	0.198	0.374	
3	5	0.040	0.190	0.209	0.467

Source: Own calculations

Thereby, the fare class number stated in the head of each column represents the fare class where a price change occurs. The corresponding elasticities of all other fare classes are displayed in the rows below the respective column.

For interpreting the results we have to keep the substitution patterns of the MNL and NL model in mind. The values of the responses to this price change are similar, though not exactly equal through aggregation, over all remaining fare classes. This indicates that a price change in the first fare class by one unit increases the choice probabilities of all other alternatives by approximately 0.1. The same way, price changes in the other fare classes are analyzed. Clearly, a change in price of the cheapest fare has the largest influence on choice probabilities. The responsiveness to a price change in a certain fare class results in similar changes of choice probabilities of all remaining fare classes. This finding again confirms constant substitution between fare classes if the behavioral process of fare class choice is assumed to be best represented by an MNL model.

Aggregate cross price elasticities of the NL model can be gathered from table 6. As substitution patterns are, by definition, not constant in the NL model the resulting NL cross price elasticities also differ from the ones obtained for the MNL model. For reasons of clarity, we add a column indicating the nest membership of each fare class. In the last four columns we have again the responses to a price change in a certain fare class. Obviously, elasticities of alternatives that are in the same nest with the alternative whose price is increased are larger in value than elasticities of alternatives that are in another nest. This indicates that substitution between fare classes within the same nest is more likely than substitution between alternatives that belong to different nests confirming the existence of the assumed correlation structure in NL error terms.

Both market shares and elasticities obtained for the generated data sets indicate that the consideration of demand dependencies for fare classes with similar characteristics may have an important impact on decisions regarding the seat inventory control in airline revenue management. Airline seat inventory control is an approach where seats are allocated to different fare classes such that revenues are maximized (Williamson, 1992, p. 28). This is done by deciding on the fare classes that are contained in each passenger's choice set. As stated above, in airline revenue management research it is common practice to assume that demand for alternatives offered at the same time is independent and does not depend on the availability of other fare classes in the choice set of a certain passenger (Talluri and Van Ryzin, 2005, pp. 33-35). Thus, by assuming that demand is best represented by an MNL model demand shifts are assumed to be proportional which may lead to an erroneous estimation of revenues in seat inventory control. Therefore, demand with constant substitution patterns is not an appropriate approach when it comes to fare class choice. As outlined in section 2.2.2 different fare classes exhibit similar restrictions that may lead to non-proportional shifts in demand when fare classes are closed for purchase. Hence, to relax the independent demand assumption demand for the seat inventory control problem in airline revenue management should be represented by a discrete choice model with non-constant substitution patterns.

4. Conclusions

In this article, we have examined the generation of synthetic data sets for fare class choice with non-constant substitution patterns. We were able to show that true coefficients of the choice problem are well recovered and lead to desired substitution patterns. Furthermore, an analysis of market shares and elasticities proves that the generated NL data set exhibits the desired correlation structure. The results provide a basis for overcoming the independent demand assumption that is usually applied in revenue management optimization models. Considering today's possibilities of accurate demand modeling with discrete choice models this assumption clearly seems to be overrun. Although the MNL model already is frequently applied in many revenue management studies it is still lacking the possibility to account for demand dependencies. It is well known that fare class restrictions can be very complex depending on the fencing desired for a particular tariff. With up to 20 different fares on a single flight restrictions might overlap for at least a few fares requiring alternate approaches of demand modeling.

Thus, our findings imply the application of more flexible discrete choice models than MNL. Especially in a combined approach for seat allocation and pricing this allows for potential revenue gains as substitution patterns differ when demand is not assumed to be independent for fare classes with similar characteristics.

One aspect that is not addressed in this article are intertemporal substitutions. In this context, the approach provided in this article can be assumed to give a cross section of passenger's choices at a certain point in time. Hence, dependencies of choice decisions at different time points are not taken into account. However, it has to be assumed that potential passengers check seat availabilities of a desired flight for a certain period of time prior to an actual booking. Passenger's decisions to not book a ticket immediately but wait for a better offer in the future also influences seat availability within the offered fare classes in the days prior to the booking. Thus, modeling intertemporal substitution by applying dynamic choice models could be an interesting approach for future research. Thereby, intertemporal dependencies of passenger choices should be modeled such that recursivity and endogeneity of passenger behavior are accounted for. Furthermore, the modeler has to keep in mind that passengers' preferences might change over time leading to dynamic inconsistency.

Abstract

The article provides a theoretical framework for the generation of synthetic discrete choice datasets for fare class choice in airline revenue management. The necessity of this research arises from simplifying assumptions regarding demand modeling that are commonly made in airline revenue management optimization models. By applying demand models with more flexible substitution patterns, like the Nested Logit (NL) model, it is possible to account for dependencies between offered fare products and their influence on airline revenue.

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