

A closed-form bounded route choice model accounting for heteroscedasticity, overlap, and choice set formation

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SHORT SUMMARY

The Multinomial Logit (MNL) model is popular in route choice modelling for its simple choice probability function. Still, it has limitations: it assumes homoscedastic error terms, ignores route overlap correlations, and assigns non-zero probabilities to all routes. We address these by developing the Bounded q-Product Logit (BqPL) model, which introduces heteroscedastic errors with bounded support. The parameter q scales error variance with trip cost, and routes exceeding a cost threshold are assigned zero probability, thus implicitly defining the choice set. We extend BqPL to capture route overlap correlations with a path size correction term, yielding the Bounded Path Size q-Product Logit (BPSqPL) model. After demonstrating the model properties on a small-scale example, it is benchmarked in a large-scale case study. The BPSqPL showed great improvements in fit and predictive ability while providing valuable insights on the non-considered routes and on how cyclists compare the different routes from a choice set.

Keywords: route choice, heteroscedasticity, route overlap, choice set formation, large-scale application

1 INTRODUCTION

The Multinomial Logit (MNL) model (McFadden, 1974) is popular in route choice applications due to its simple closed-form choice probabilities. However, MNL relies on several assumptions that limit its behavioral realism:

- *Homoscedasticity:* MNL assumes identical variance for error terms across all routes, which may be unrealistic in many contexts (Bhat, 1995; Munizaga et al., 2000).
- *Independence:* MNL assumes uncorrelated error terms, yet routes often overlap, sharing links and unobserved attributes (Cascetta et al., 1996; Ben-Akiva & Bierlaire, 1999).
- *Non-bounded support:* MNL assumes that each alternative has a non-zero choice probability, disregarding choice set formation and leading to potential biases (Horowitz & Louviere, 1995; Williams & Ortuzar, 1982).

Several models have emerged to address these limitations individually, including approaches for heteroscedasticity (Bhat, 1995; Castillo et al., 2008; Chikaraishi & Nakayama, 2016), route overlap (Vovsha, 1997; Cascetta et al., 1996; Ben-Akiva & Bierlaire, 1999), and alternative non-consideration has been addressed in various way, such as using two-stage models (Manski, 1977), one-stage approximations (Cascetta & Papola, 2001), or bounded-support probability distributions (Watling et al., 2018; Tan et al., 2024). However, few models address multiple limitations simultaneously. For example, the Path Size Weibit (Kitthamkesorn & Chen, 2013) model handles both heteroscedasticity and correlation, while the Bounded Path Size Logit (Duncan et al., 2022) addresses overlap and choice set formation. To our knowledge, no model addresses these three

limitation simultaneously, which is mainly due to confounding effects (Hess & Train, 2017) and poor scalability of some of the above-mentioned methods to large-scale problems such as route choice.

In this paper, we introduce a new model that unifies these elements. Building on the q-Product Logit (qPL) (Chikaraishi & Nakayama, 2016) and Bounded Logit (BL) (Watling et al., 2018) models, we develop the Bounded Path Size q-Product Logit (BPSqPL). This model integrates bounded choice sets, heteroscedasticity, and route correlation, offering a flexible framework that encompasses multiple existing models.

2 METHODS

Let us assume that we observe a choice situation with choice set \mathcal{C} . We assume that each observation can be described by a **positive** random cost function C_i^1 , which both depends on observed attributes, aggregated in a deterministic cost c_i , and a random error term ϵ_i . While logit models assume a $C_i = c_i + \epsilon_i$ and weibit models assume $C_i = c_i \epsilon_i$, we will present the concept of "q-generalisation", allowing the relation between deterministic and random cost components to be between the sum and product. This concept is at the core of Chikaraishi & Nakayama (2016) derivation of the qPL model, as well as our BqPL model.

q-Generalisation

Here, we present some q-operators. First, the "q-product" (Borges (2004)) can be seen as an in-between of the sum and the product. The $q \in [0, 1]$ parameter controls the closeness to the sum or product. It is defined for $a > 0$ and $b > 0$ such that $a^{1-q} + b^{1-q} - 1 > 0$ as:

$$a \otimes_q b = (a^{1-q} + b^{1-q} - 1)_+^{\frac{1}{1-q}} \quad (1)$$

where $(\cdot)_+ = \max(0, \cdot)$. Its limiting cases are $\lim_{q \rightarrow 1} a \otimes_q b = ab$ and $a \otimes_0 b = a + b - 1$. We can similarly define the "q-ratio" as the inverse operator of the q-product:

$$a \oslash_q b = (a^{1-q} - b^{1-q} + 1)_+^{\frac{1}{1-q}} \quad (2)$$

Its limiting cases are $\lim_{q \rightarrow 1} a \oslash_q b = a/b$ and $a \oslash_0 b = a - b + 1$. It is the inverse of the q-product because $a \otimes_q (1 \oslash_q a) = 1$. Additionally, for any positive real number x , we define the "q-logarithm" (Tsallis (1994)) as:

$$\ln_q(x) = \begin{cases} \frac{x^{1-q} - 1}{1-q} & \text{if } q \neq 1 \\ \ln(x) & \text{if } q = 1 \end{cases} \quad (3)$$

Notably, $\ln_0(x) = x - 1$. We have that $\ln_q(a \otimes_q b) = \ln_q(a) + \ln_q(b)$. Additionally, we define the q-LogLogistic distribution as follows:

$$F_Z(x) = F_{qL}(x|\theta, \mu, q) := \frac{1}{1 + \exp[-\theta(\ln_q(x) - \ln_q(\mu_Z))]} \quad (4)$$

Chikaraishi & Nakayama (2016) derives the qPL model by assuming that, for each alternative i , $C_i = c_i \otimes_q \epsilon_i$, where $\ln_q(\epsilon_i)$ follow independent Gumbel distributions. This assumption implies that the error term q-Ratio between any two alternatives $\epsilon_i \oslash_q \epsilon_j$ follows the q-LogLogistic distribution defined in Equation 4. We use a similar assumption to derive the BqPL model, with the difference that we use a left-truncated distribution.

Derivation of the Bounded q-Product Logit model

Analogously to Watling et al. (2018)'s BL model, we assume that individuals compare each alternative $i \in \mathcal{C}$ to an imaginary reference alternative r^* in terms of utility q-Ratio:

$$C_i \oslash_q C_{r^*} = (c_i \otimes_q \epsilon_i) \oslash_q (c_{r^*} \otimes_q \epsilon_{r^*}) = c_i \oslash_q c_{r^*} \otimes_q \epsilon_i \oslash_q \epsilon_{r^*} = c_i \oslash_q c_{r^*} \otimes_q \varepsilon_i$$

¹The model can be equally be derived for utility maximization and cost minimization

The proposed Truncated q-Log-Logistic distribution is derived by left-truncating the q-Log-Logistic distribution at a lower bound $1 \oslash_q \phi$ for some $\phi \geq 1$. The following PDF defines it:

$$f_{qT}(x|\theta, \mu, q, \phi) = \begin{cases} \frac{f_{qL}(x|\theta, \mu, q)}{1 - F_{qL}(1 \oslash_q \phi|\theta, \mu, q)} & \text{if } x \geq 1 \oslash_q \phi \\ 0 & \text{if } 0 \leq x < 1 \oslash_q \phi \end{cases} \quad (5)$$

The BqPL choice probabilities can be obtained from this assumption, and are defined by:

$$P_i^{\text{BqPL}} := \Pr(i|\mathcal{C}) = \frac{(e^{-\theta \ln_q(c_i \oslash_q (\phi \otimes_q c_{r^*}))} - 1)_+}{\sum_{j \in \mathcal{C}} (e^{-\theta \ln_q(c_j \oslash_q (\phi \otimes_q c_{r^*}))} - 1)_+} \quad (6)$$

Accounting for route overlap

To account for route overlap, we take inspiration from the Bounded Path Size Logit (BPSL) model (Duncan et al., 2022) to formulate a Bounded Path Size q-Product Logit (BPSqPL) model, where the path size terms are defined appropriately to capture correlations between considered routes only and a continuous choice probability function is maintained. Each route $i \in \mathcal{C}$ consists of a set of links $A_i \subseteq A$, where A is the universal set of links in the network. These links are defined by attributes aggregated in positive cost functions $t_a, a \in A$, parameterised by a vector of parameters α . The total cost c_i of route i is link-additive, i.e. $c_i = \sum_{a \in A_i} t_a$. The BPSqPL choice probability function for route i is:

$$P_i^{\text{BPSqPL}} = \frac{(\gamma_i^{\text{BPSqPL}})^\eta \left(\exp(-\theta(\ln_q(c_i) - \ln_q(\varphi \min_{l \in \mathcal{C}} c_l))) - 1 \right)_+}{\sum_{j \in \mathcal{C}} (\gamma_j^{\text{BPSqPL}})^\eta \left(\exp(-\theta(\ln_q(c_j) - \ln_q(\varphi \min_{l \in \mathcal{C}} c_l))) - 1 \right)_+} \quad (7)$$

where $(\gamma_i^{\text{BPSqPL}})^\eta$ is the path size correction factor for considered route $i \in \mathcal{C}$. $\eta \geq 0$ is the path size scaling parameter scaling sensitivity to route distinctiveness, and $\gamma_i^{\text{BPSqPL}} \in [0, 1]$ is calculated as follows:

$$\gamma_i^{\text{BPSqPL}} = \sum_{a \in A_i} \frac{t_a}{c_i} \frac{w_i}{\sum_{j \in \mathcal{C}} w_j \delta_{aj}} \quad (8)$$

$w_i = \left(\exp(-\theta(\ln_q(c_i) - \ln_q(\varphi \min_{l \in \mathcal{C}} c_l))) - 1 \right)_+$ is the weight of route i in the Path-Size contribution of all the other routes, proportional to its choice probability. This model generalizes Ben-Akiva & Bierlaire (1999) correction, which sets $w_i = 1, \forall i$. Hence, γ_i^{BPSqPL} is specified so that a) routes with costs above the bound do not contribute to reducing the path size terms of routes with costs below the bound, and b) the path size term function is continuous as routes enter and exit the considered route set.

Special cases of the BPSqPL

Both the BqPL and BPSqPL are generalizations of some existing (and new) choice models. For $q = 1$, the BqPL (respectively, the BPSqPL) collapse to what we define as the Bounded Weibit (BW) (respectively, the Bounded Path Size Weibit (BPSW), which extend Castillo et al. (2008) Multinomial Weibit (MNW). For $q = 0$, the models respectively collapse to the BL and BPSL. When the bound φ tends to $+\infty$, the bounded models tend to their unbounded counterparts. The BPSqPL thus unifies several modelling frameworks.

Example

We demonstrate the features of the BPSqPL model and its variations on a test network (Figure 1), which includes seven links with costs defined by parameters $\lambda > 0$ and $0 < \rho < \lambda$. These links form five routes between O and D, detailed in Table 1. A key feature of this network is that Route 3 is correlated with Route 4, which becomes less preferable as ρ grows. This setup illustrates the differences between the BPSx (BPSW/BPSL/BPSqPL) correction and the commonly used Path size correction from Ben-Akiva & Bierlaire (1999).

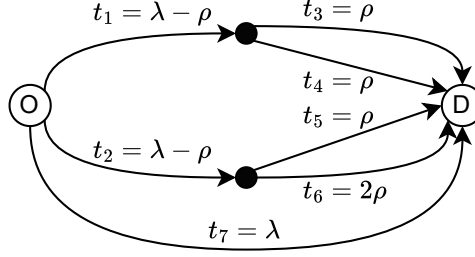


Fig. 1: Toy network with 7 links and 5 routes

Route	Links	Cost
1	1-3	λ
2	1-4	λ
3	2-5	λ
4	2-6	$\lambda + \rho$
5	7	λ

Tab. 1: Set of routes using the network from Figure 1

We plot the choice probabilities of each alternative in Figures 3 and 2 as a function of the ratio ρ/λ , which ranges from 0 to 1. This ratio indicates how distinct Routes 1 to 4 are from each other (0 means fully confounded; 1 means fully distinct). We use two values for λ ($\lambda = 1$ and $\lambda = 10$) to represent short and long trips.

Figure 3 shows the choice probabilities for models without Path size correction or bounding ((a), (b), and (c)) and for a bounded model without Path size correction (BqPL, (d)). For $\lambda = 1$, MNL, MNW, and qPL models have similar choice probabilities. As ρ increases, Route 4 becomes less competitive, reducing its choice probability. When $\lambda = 10$, the three models diverge: MNL (Figure 3 (a)) shows a sharper decrease for Route 4 due to cost sensitivity, while MNW (Figure 3 (b)) remains unaffected by scale, focusing on cost ratios alone. The qPL (Figure 3 (c)) balances between MNL and MNW, responding to the cost q-Ratio. The BqPL model (Figure 3 (d)) behaves similarly to qPL but assigns zero probability to Route 4 once it reaches the relative cost bound ($\rho = 0.8\lambda$), increasing the choice probability gradient compared to qPL. In all cases, Routes 1, 2, 3, and 5 share the same probability regardless of overlap.

Figure 2 addresses this limitation with the BPSqPL model, which includes Path size correction. In Figure 2 (a), the BqPL-PS model uses a correction term that penalizes utility without depending on route cost. Route 5 has the highest choice probability due to minimal overlap with other routes. However, Route 3 receives the same penalty as Routes 1 and 2, even if it overlaps with a less realistic option, a standard Path size correction limitation, as noted by Duncan et al. (2020). The BPSqPL model (Figure 2 (b)) improves this by assigning Route 5 the highest probability, given its distinctness. When $\rho = 0$, Routes 1 and 2 and Routes 3 and 4 are confounded and share split probabilities. As ρ increases, Route 4's probability decreases, while Route 3 converges with Route 5, which has no overlaps. When $\rho > 0.8\lambda$, Route 4's cost exceeds the bound, resulting in a zero probability, and Route 3 aligns with Route 5's probability due to the lack of overlap.

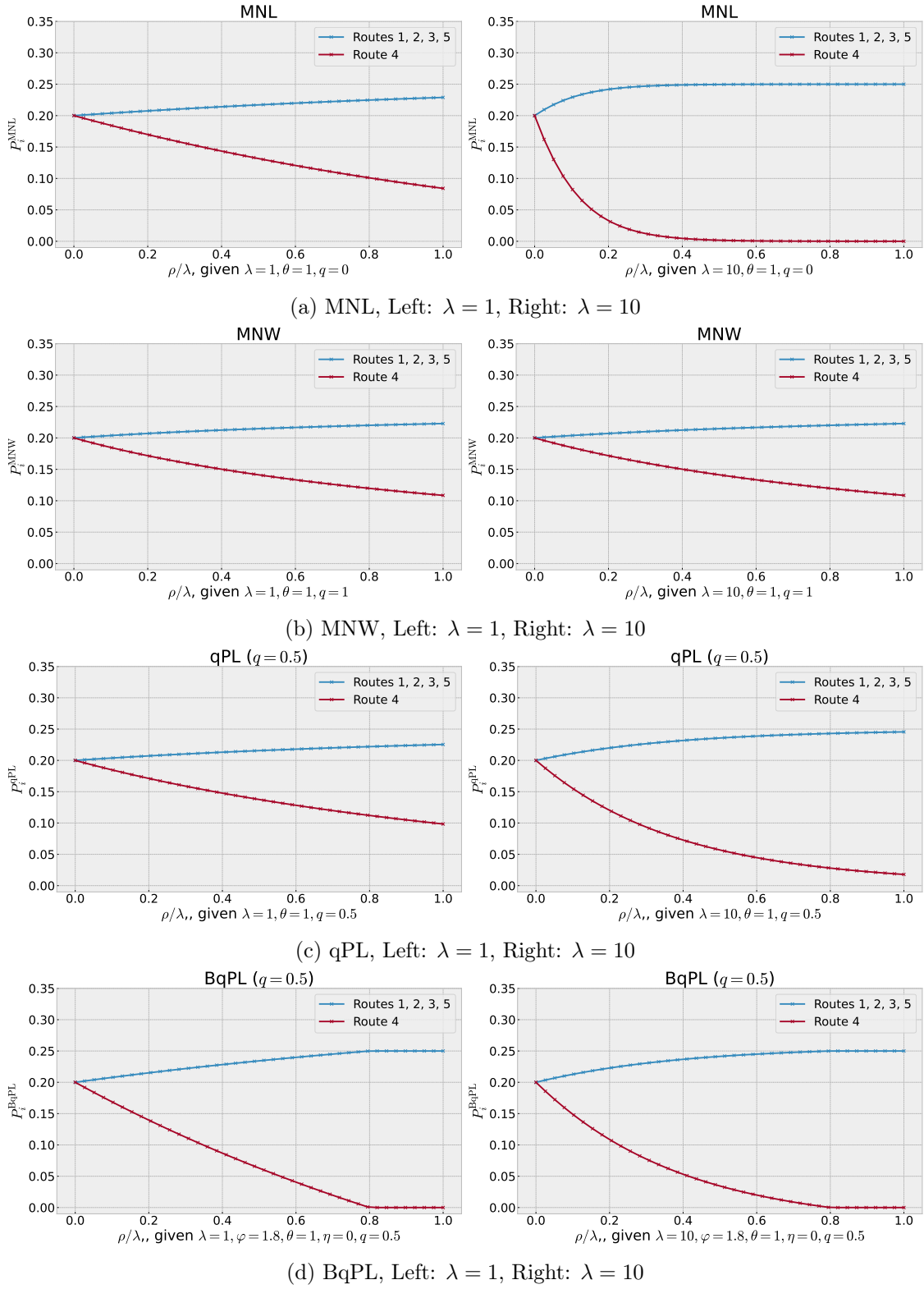


Fig. 2: Choice probabilities as a function of ρ on the example network from Figure 1.

3 CASE STUDY

The case utilised a large-scale crowd-sourced data set of bicycle GPS trajectories received from Høvdning. The original dataset covers the entire Greater Copenhagen Area from the 16th September 2019 until 31st May 2021. For a detailed description of the data, the bicycle network, and the algorithms applied for data processing, we refer to [Lukawska et al. \(2023\)](#). The final dataset for model estimation consists of a subset of this dataset containing 4,134 trips made by 4,134 cyclists. For a detailed description of the choice set generation technique, and the model specification, the

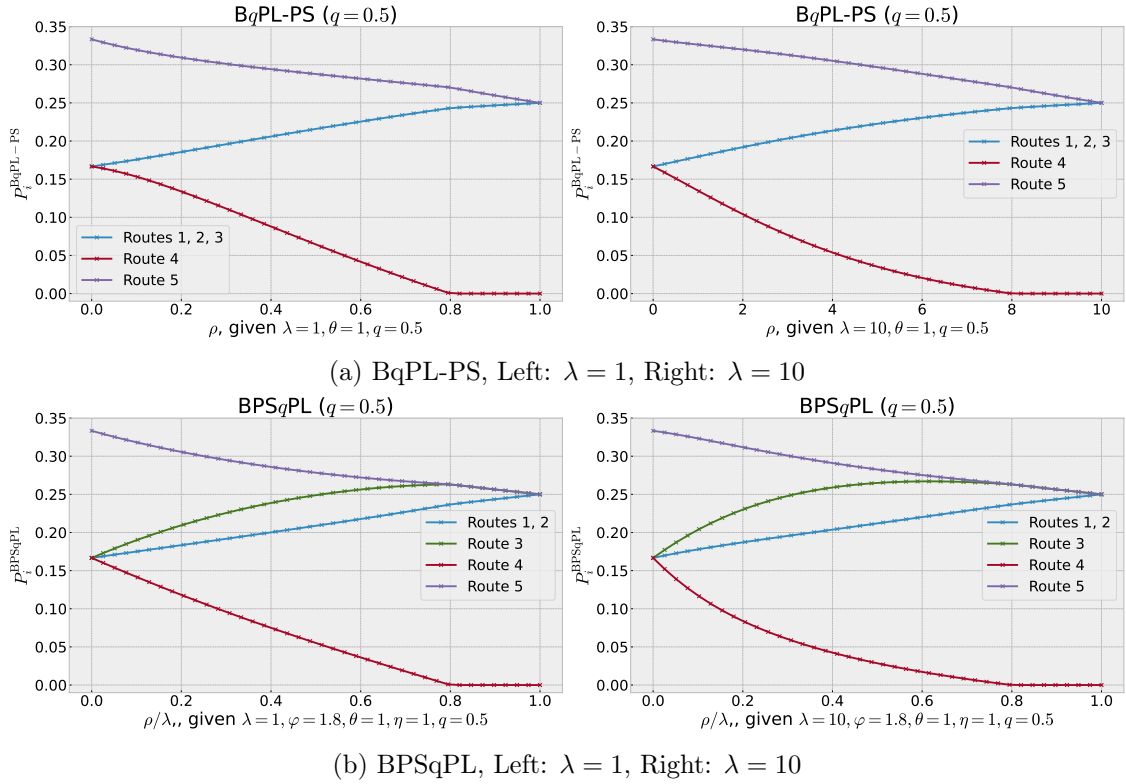


Fig. 3: Choice probabilities as a function of ρ on the example network from Figure 1.

reader is referred to [Cazor et al. \(2024\)](#).

Estimation results

The results are presented in Table 2, which comprise the BPSqPL and some of its special cases: the MNL, qPL, BL, BqPL, BPSL. Moreover, the BqPL-PS was presented, using [Ben-Akiva & Bierlaire \(1999\)](#), to compare this alternative correction. All the estimated parameters were significant at the 0.01 level. Each extension of the MNL and its one additional parameter significantly affects model fit, which can be seen in a decrease in the BIC for the more complex models.

We make the following observations:

- The qPL, BqPL and BPSqPL all estimate a q parameter significantly different from 0 and 1, inducing heteroscedasticity in the route costs. This suggests that cyclists are neither sensitive to route cost differences nor ratios but something in-between (closer to the ratio, though, as q ranges between 0.562 and 0.706).
- For the bounded models that incorporate choice set formation (Table ??), the relative cost bound is consistent across models, estimated between 1.102 and 1.162. This implies that cyclists rarely considered routes more than 10.2–16.2% costlier than the cheapest option. Non-considered routes (those with zero probability) accounted for 41.9–68.5% of the pre-generated routes, indicating that the choice-set generation method included a substantial number of behaviorally unrealistic routes.
- The scale is the only parameter that varies between models, while the taste parameters are rather stable. The different scales are linked to the different assumed distributions for the error terms (Gumbel, q-Gumbel or Weibull), whose variance behaves differently when route length increases. Overall, This implies that accounting for heteroscedasticity, choice set formation, and alternative correlation does not change the taste interpretation (at least in this dataset) but is of good value for getting closer to realistic substitution patterns between routes and more reliable forecasting.
- Notably, when comparing Path size specifications, the more advanced and consistent one greatly improves the fit (BPSqPL vs. BqPL-PS). This suggests that this weighting is more behaviorally realistic.

Model	MNL	qPL	BL	BqPL	BPSL	BPSqPL	BqPL-PS
Length	-	-	-	-	-	-	-
Elevation gain	0.00352	0.00658	0.0031	0.00616	0.0036	0.00438	0.0045
No Bike infrastructure	0.182	0.183	0.17	0.181	0.159	0.155	0.151
Non-smooth surface	0.194	0.2	0.171	0.198	0.153	0.153	0.16
Wrong way	0.332	0.358	0.31	0.356	0.267	0.262	0.296
Scale (θ)	-28.5	-51.76	-25.42	-50.5	-14.71	-28.56	-58.68
Path size term (η)	-	-	-	-	1.643	1.571	1.122
q	-	0.706	-	0.688	-	0.562	0.67
Relative cost bound (φ)	-	-	1.111	1.149	1.105	1.115	1.126
Final LL	-11,087	-10,363	-10,791	-10,357	-9,910	-9,683	-10,163
BIC	22,192	20,748	21,604	20,739	19,845	19,395	20,355
Adj. ρ^2	0.513	0.545	0.526	0.545	0.565	0.575	0.554
N. of parameters	5	6	6	7	7	8	8
% of routes cut by φ	-	-	66.3%	53.4%	65.7%	60.3%	56.8%

Tab. 2: Model estimates for selected models

Model validation

We performed Monte-Carlo cross-validation on our dataset to assess the model’s predictive performance and test for overfitting. To do so, we repeated $N = 10$ (as in [Cazor et al. \(2024\)](#)) times the following steps:

1. Randomly split the original dataset S into a training S_t and validation set S_v ($|S_t| = 0.7|S|$; $|S_v| = 0.3|S|$).
2. Estimate all the models on the training set S_t , obtain, for each model m , the training parameters β_m^t .
3. Calculate, for each model m , the log-likelihood on the validation set, $LL = \sum_{x \in S_v} \log P_{i_x}^m(\beta_m^t)$, where i_x is the index of the chosen alternative for observation $x \in S_v$.

The cross-validation results are shown in Table 3. The BPSqPL is the best-performing model in every cross-validation experiment, followed by the BPSL, the BqPL, the qPL, the BL and the MNL. This indicates that these models did not overfit the data. Moreover, we observed that the model estimates across the experiments were stable.

Model	MNL	qPL	BL	BqPL	BPSL	BPSqPL
Average LL	-3,217.48	-3,009.63	-3,107.61	-3,005.12	-2,872.35	-2,817.81

Tab. 3: Average log-likelihood on the cross-validation sets

4 CONCLUSION

In this paper, we have developed new closed-form choice models that generalise the MNL to account for heteroscedasticity of the error terms, correlations between overlapping routes, and choice set formation effects through setting a bound on the relative cost distribution. We first developed a model that combines [Chikaraishi & Nakayama \(2016\)](#)’s q-Product Logit (qPL) model with [Watling et al. \(2018\)](#)’s Bounded Logit (BL) model, to derive a Bounded q-Product Logit (BqPL) model. It is derived by assuming a Truncated q-Log-Logistic distribution for random error term differences and can be seen as a one-stage choice set formation model. We then extended the BqPL model to account for route overlap in a fashion similar to [Duncan et al. \(2022\)](#)’s BPSL model.

The BPSqPL model remains parsimonious and easy to estimate by introducing only one additional parameter per property. This model unifies several frameworks and generalises several known and new models. Model properties were first demonstrated using a small-scale example and then benchmarked against existing models in a large-scale bicycle route choice case study.

Our findings from the large-scale application show that accounting for heteroscedasticity, route overlap, and choice set formation considerably improves model fit and predictive accuracy. The estimate for the q parameter also indicates that error term variance does increase with expected route cost but is slightly slower than the quadratic increase assumed by a Weibit model. These enhancements were achieved without a substantial increase in model complexity. Additionally, these models offer more realistic substitution patterns between alternatives due to consistent path size corrections and the exclusion of unrealistic alternatives, which account for about 50% of the generated representative universal choice set of routes. The values of the taste coefficients for the observed attributes also remained stable across models.

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