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# A bounded path size route choice model excluding unrealistic routes: Formulation and estimation from a large-scale GPS study

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**Abstract**

This paper develops a new route choice modelling framework that deals with both route correlations and unrealistic routes in a consistent and robust way. To do this, we explore the integration of a correlation-based Path Size Logit model with the Bounded Choice Model (BCM) (Watling et al, 2018). We find, however, that the natural integration of these models leads to behavioural inconsistencies and/or undesirable mathematical properties. Solving these challenges, we derive a mathematically well-defined Bounded Path Size (BPS) model form that utilises a consistent criterion for assigning zero choice probabilities to unrealistic routes while eliminating their path size contributions. Two BPS models are consequently formulated: one that is closed-form and another expressed as a fixed-point problem. Subsequently, we consider parameter estimation in a simulation study and on a real-life large-scale network using GPS data, where computational feasibility is demonstrated. Estimation results show the potential of the BPS models to give improved fit relative to non-bounded versions (as well as the BCM), while providing greater robustness to the assumed choice sets.

**Key Words:** bounded choice model, path size logit, route choice, parameter estimation, unrealistic routes

## 1 Introduction

There are several distinct and unique aspects about route choice modelling that makes it a more challenging task than modelling other types of transport choices. Two key aspects are that: 1) there is often a complex correlation structure between the route alternatives, which occurs due to the significant topological overlapping of routes; and 2) typical road networks have many possibilities for very long routes that should be considered unrealistic and excluded from route choice. To the best knowledge of the authors, no route choice modelling approach has been developed thus far that addresses both of these challenges in a theoretically consistent, robust, and mathematically well-defined way, and that moreover, has been shown to be both computationally feasible in large-scale networks and estimatable from revealed choice data. In this paper, we aim to address this by developing a new model framework. To set the background for the research, below, we discuss modelling approaches for 1) and 2), and how we decided upon the approach taken.

To overcome the deficiency of the Multinomial Logit (MNL) Random Utility Model (RUM) in its inability to capture correlations between routes, numerous MNL extension models have been proposed that relax the assumption that the random error terms are independently distributed. Alternative RUMs to MNL either capture route correlations implicitly or utilise concepts from extended Logit models to similarly adapt the model. For a more detailed review, see Duncan et al (2020); however, we discuss the key models and concepts relevant to this paper below:

- GEV structure models use a multi-level tree structure to capture the similarity among routes through the random error component of the utility function. Such models include: Cross-Nested Logit (CNL) (Vovsha, 1997; Bekhor & Prashker, 1999; Marzano & Papola, 2008), Paired Combinatorial Logit (Chu, 1989; Bekhor & Prashker, 1999; Gliebe et al, 1999; Pravinvongvuth & Chen, 2005), Generalized Nested Logit (GNL) (Bekhor & Prashker, 2001; Wen & Koppelman, 2001), and the Network GEV model (Bierlaire, 2002; Daly & Bierlaire, 2006).
- Simulation models include Mixed Logit models (Ben-Akiva & Bolduc, 1996; McFadden & Train, 2000) such as the Factor Analytic Logit Kernel model (Bekhor et al, 2002), as well as alternative RUMs to MNL such as Multinomial Probit (MNP) (Daganzo & Sheffi, 1977) and Multinomial Gammit (MNG) (Cantarella & Binetti,

2002). Mixed Logit models divide the error terms into two Gumbel and Gaussian distributed variable components which ensures the Logit structure is kept while allowing for capturing interdependencies between routes. MNP and MNG etc. do not suffer from the same issue as MNL, as the similarity between each pair of routes is accounted for by allowing for covariance between the error terms, and route correlations are thus captured implicitly.

- Correction term models add correction terms to the deterministic utilities / probability relations to adjust the choice probabilities in order to capture route correlations. Such models include: C-Logit (CL) (Cascetta et al, 1996), Path Size Correction Logit (PSCL) (Bovy et al, 2008), Path Size Logit (PSL) (Ben-Akiva & Ramming, 1998), Path Size Hybrid (Xu et al, 2015), and Path Size Weibit (Kitthamkesorn & Chen, 2013).

The typical route choice modelling approach for dealing with unrealistic routes – for correlation-based models and in general – is to employ some kind of heuristic method that attempts to explicitly generate a route choice set containing just the routes considered realistic. This approach, however, leads to theoretical inconsistencies, since the route generation criteria is not consistent with the calculation of the choice probabilities among chosen routes. Moreover, in large-scale case studies, for example the study of eastern Denmark in Prato et al (2014), Rasmussen et al (2017), Duncan et al (2020), as well as in Section 7.4 of this paper, it is implausible to attempt to generate the exact choice sets of realistic routes, and instead choice sets are generated large enough so that one can be fairly certain the realistic alternatives are present, regardless of how many unrealistic routes are generated. This is problematic, since many correlation-based models are not choice set robust, and results are thus negatively influenced by the presence of the unrealistic routes as well as highly sensitive to the choice set generation method adopted (Bovy et al, 2008; Bliemer & Bovy, 2008; Ramming, 2002; Ben-Akiva & Bierlaire, 1999; Bekhor et al (2008); Duncan et al, 2020).

An approach that has recently been proposed for consistently dealing with unrealistic routes is the Bounded Choice Model (BCM) (Watling et al, 2018). The BCM has a consistent criterion for determining restricted choice sets of realistic routes, and route choice probability: a bound is applied to the difference in random utility between each given route and an imaginary reference route alternative, so that routes only receive a non-zero choice probability if the difference between its random utility and the random utility of the reference alternative is within the bound. Furthermore, the probability by which each route is chosen relates to the odds associated with choosing each alternative versus the reference alternative. A special case of the BCM is where the reference alternative is that with the maximum deterministic utility i.e. the route with the cheapest generalised travel cost, so that a route only receives a non-zero probability if its cost is within some bound of the cheapest route.

The BCM does not account for route correlation however, and motivated by the desire to develop a route choice model that deals with both route correlation and unrealistic routes in a consistent and robust way, an approach we deemed promising was to explore the integration of a correlation-based model with the BCM. To determine which correlation-based model we would adopt, there were requirements: real-life application of a route choice model involves estimating the model parameters, and we thus considered it important that the proposed model could be successfully estimated, and moreover, that it would be computationally feasible to do so on large-scale networks. Below, we consider the suitability of the correlation-based model categories in terms of potential to satisfy these requirements.

For GEV structure and simulation models, there are computational concerns: computing route choice probabilities / estimation typically requires a high computational cost on large-scale networks. Although GEV structure models have closed-form probability expressions, due to their multi-level tree structure the choice probabilities are complex to compute, where the computational burden escalates significantly as the scale of network / choice set sizes increase. This raises concerns over their applicability to large-scale networks. For example, Lai & Bierlaire (2015) estimate CNL on a medium-scale network and find significantly greater computation times than for MNL/PSL (e.g. 9.76 hours compared to 98.7/116 seconds). The problem for simulation models is that they do not have closed-form expressions and solving the choice probabilities requires either Monte Carlo simulation or alternative methods, all of which are computationally burdensome. Many analytical approximation methods have been proposed to solve the MNP model, all aiming to provide the best compromise between speed and accuracy (reviews can be seen in e.g. Rosa (2003), Connors et al (2014)); however, performance of these approaches are assessed with a very limited number of routes, typically up to just 25 alternatives. It is generally considered infeasible to accurately compute MNP, MNG etc. probabilities on large-scale networks with thousands of routes.

There are also estimation concerns for GEV structure and simulation models: numerous studies have found/discussed difficulties in obtaining reasonable estimates for parameters. There are numerous different issues involved in estimating the numerous different specifications of the CNL model for route choice, and several studies have discussed issues in detail, for example see Bierlaire (2006), Abbe et al (2007), Marzano & Papola (2008). To summarise a few of the issues documented: a) there may be infinite specifications with different choice probabilities that lead to the same covariance figures (Marzano & Papola, 2008); b) the number of unknown parameters to be estimated increases as the number of routes increases (Marzano & Papola, 2008); c) several studies have found that when estimating the nesting coefficients the model tends to collapse to MNL (Ramming, 2002; Prato, 2005; Prato & Bekhor, 2006); d) the maximum likelihood estimation functions are not concave which significantly complicates the identification of a global maximum (Bierlaire, 2006); and, e) because of d), nonlinear programming methods tend to converge towards local maxima of the log-likelihood function, and in practice, one observes a significant influence of the initial values provided to the algorithm on the estimated parameters (Abbe et al, 2007). GNL requires the estimation of an additional parameter over CNL which makes parameter estimation more difficult. There are also difficulties in estimating the parameters of the Factor Analytic Logit Kernel model: Ramming (2002) finds instable estimates of the covariance parameters, despite the very large number of random draws, while Prato (2005) discusses the difficulty in obtaining significant estimates. And, there are also issues involved in estimating the MNP model, including: identification issues arising from the number of parameters that may need to be estimated (Dansie, 1985; Bunch, 1991; Keane, 1992); and, difficulties in accurately computing small choice probabilities (Connors et al, 2014).

Correction term models are in contrast much more computationally practical than GEV structure and simulation models, and are regularly applied and estimated on large-scale networks. They have simple closed-form expressions, meaning the route choice probabilities are generally easy and quick to compute. They are thus a useful and practical approach to approximating the correlation; more complex models can capture the correlation more accurately, but due to the comparatively low computational cost and the relative ease in obtaining reasonable estimates for parameters, correction term models are the most commonly used models in practice.

Motivated by the above, we decided to explore the integration of a correction term model with the BCM. The CL model proposes that the correction terms are based upon commonality factors that measure the similarity of routes, and penalises the utilities accordingly. In contrast, the PSL model proposes that the correction terms are based upon path size terms that measure route distinctiveness: a route is penalised based on the number of other routes sharing its links, and the costs of those shared links. The PSCL model provides a modified path size term derived from an approximation of GEV models.

Developing a BCM with an integrated correction term was complicated by the desire to produce a model such that the correction terms consistently and only capture correlations between the routes the model defines as realistic. Achieving this, however, and maintaining a continuous choice probability function is far from trivial, as the research in this paper shows. Continuity is an important property, and is typically required for applications of the model that are well-behaved, for example convergent parameter estimation and existence of network equilibria. Thus, when considering which correction term model to integrate we considered how continuity could be achieved. We found that while one can derive a BCM with an integrated CL correction term, there are uncertainties over how one can suitably maintain a continuous probability function. For the PSL model, existing research on dealing with unrealistic routes within the path size terms presented a clear direction to pursue, and while similar techniques could be translated for the PSCL model, PSL is much more widely used and we therefore chose to pursue developing a BCM with an integrated PSL-like correction term.

The pragmatic approach that has been proposed for addressing choice set robustness for PSL, is to utilise a weighted path size contribution technique along with choice set generation, to reduce the negative effects of any present unrealistic routes. The Generalised Path Size Logit (GPSL) model (Ramming, 2002) proposes a path size contribution factor based on travel cost ratios to reduce the contributions of costly routes, while the Adaptive Path Size Logit (APSL) model (Duncan et al, 2020) proposes a contribution factor based on choice probability ratios to provide internal consistency. While improving upon the choice set robustness of PSL, these approaches do not solve the issue entirely since the path size contributions of routes defined as unrealistic are only reduced instead of eliminated.

Taking the promising weighted path size contribution approach one step further, by integrating PSL concepts with the BCM, the aim is to develop a model that eliminates unrealistic route contributions entirely, as well as removing all the negative effects of unrealistic routes by also assigning them zero choice probabilities. A natural form for a Bounded Path Size (BPS) model can be derived by inserting path size choice model utilities into the standard BCM formula. However, as we show, this natural form for a BPS model is deeply problematic and there are no behaviourally and practically desirable formulations. This is because appropriately defining the path size contribution factors within the path size terms is challenging, and from demonstrating with different options we establish desired properties for a theoretically consistent, robust, and mathematically well-defined BPS model. To develop a BPS model that satisfies these properties, we then derive an alternative BPS model form and consequently propose two BPS models: one that is closed-form and another expressed as a fixed-point problem.

The structure of the paper is as follows. In Section 2 we introduce some basic network notation as well as the definitions of relevant models. In Section 3 we discuss issues with the natural form for a BPS model and consequent desired properties for a BPS model (demonstrated in detail in Appendix C), and derive an alternative BPS model form. In Sections 4&5 we propose two BPS models adopting the alternative form. We also in Section 5 provide a solution method for computing the choice probabilities, which are a solution to a fixed-point problem, and address the existence and uniqueness of solutions (where the proofs are given in Appendix D). In Section 6 we discuss/demonstrate the theoretical properties of the proposed BPS models including how they satisfy the desired properties (demonstrated in detail in Appendix E). In Section 7 we investigate parameter estimation. To show that the model parameters can be estimated we first propose a Maximum Likelihood Estimation procedure for estimation with tracked route observation data, then investigate this procedure in simulation studies on the Sioux Falls network where we show that it is generally possible to reproduce assumed true parameters. Then, in a real-life case study, we estimate the BPS models using real tracked route

GPS data on a large-scale network, compare results with other models, and assess computational feasibility. Section 8 concludes the paper.

# 2 Notation & Model Definitions

## 2.1 Basic Network Notation

The model developed in this paper is applicable to general networks with multiple OD movements and flow-dependent link costs. However, without compromising the model derivation, we simplify notation by considering a single OD movement with fixed link costs. The network consists of link set $A$. For the OD movement, $R$ is the choice set of all simple routes (without cycles), having size $N = |R|$. $A_i \subseteq A$ is the set of links belonging to route $i \in R$, and $\delta_{a,i} = \begin{cases} 1 & if\ a \in A_i \\ 0 & otherwise \end{cases}$. Suppose that the generalised travel cost $t_a$ of each link $a \in A$ is a weighted sum (by parameter vector $\boldsymbol{\alpha}$) of variables $\boldsymbol{w}_a$, i.e. $t_a(\boldsymbol{w}_a; \boldsymbol{\alpha})$, and that the generalised travel cost for route $i \in R$, $c_i$, can be attained through summing up the total cost of its links so that $c_i\big(\boldsymbol{t}(\boldsymbol{w}; \boldsymbol{\alpha})\big) = \sum_{a\in A_i} t_a(\boldsymbol{w}_a; \boldsymbol{\alpha})$, where $\boldsymbol{t}$ is the vector of all link travel costs and $\boldsymbol{w}$ is the vector of all link variables. To simplify notation $c_i\big(\boldsymbol{t}(\boldsymbol{w}; \boldsymbol{\alpha})\big)$ is denoted just as $c_i$. The route choice probability for route $i \in R$ is $P_i$, where $\boldsymbol{P} = (P_1, P_2, \dots, P_N)$ is the vector of route choice probabilities, and $D$ is the set of all possible route choice probability vectors:

$$D = \left\{\boldsymbol{P} \in \mathbb{R}^N_{\geq 0} : 0 \leq P_i \leq 1, \forall i \in R, \sum\nolimits_{j=1}^{N} P_j = 1\right\}.$$

And, $D^{>0} \subset D$ is the subset of all possible route choice probability vectors where no route has zero choice probability:

$$D^{>0} = \left\{\boldsymbol{P} \in \mathbb{R}^N_{>0} : 0 < P_i < 1, \forall i \in R, \sum\nolimits_{j=1}^{N} P_j = 1\right\}.$$

## 2.2 Path Size Logit Models

Path Size Logit models were developed to address the well-known deficiency of the Multinomial Logit (MNL) model in its inability to capture the correlation between routes. To do this, they include correction terms to penalise routes that share links with other routes, so that the deterministic utility of route $i \in R$ is $V_i = -\theta c_i + \kappa_i$, where $\theta > 0$ is the Logit scaling parameter and $\kappa_i \leq 0$ is the correction term for route $i \in R$. The choice probability for route $i \in R$ is:

$$P_i = \frac{e^{-\theta c_i + \kappa_i}}{\sum_{j\in R} e^{-\theta c_j + \kappa_j}}.$$

Path Size Logit correction terms adopt the form $\kappa_i = \beta \ln(\gamma_i)$, where $\beta \geq 0$ is the path size scaling parameter, and $\gamma_i \in (0,1]$ is the path size term for route $i \in R$. A distinct route with no shared links has a path size term equal to 1, resulting in no penalisation. Less distinct routes have smaller path size terms and incur greater penalisation. The choice probability for route $i \in R$ is thus:

$$P_i = \frac{e^{-\theta c_i + \beta \ln(\gamma_i)}}{\sum_{j\in R} e^{-\theta c_j + \beta \ln(\gamma_j)}} = \frac{(\gamma_i)^\beta e^{-\theta c_i}}{\sum_{j\in R} (\gamma_j)^\beta e^{-\theta c_j}}. \tag{1}$$

The general form for the path size term is as follows:

$$\gamma_i = \sum\nolimits_{a\in A_i} \frac{t_a}{c_i} \frac{1}{\sum_{k\in R} \left(\frac{W_k}{W_i}\right) \delta_{a,k}}, \tag{2}$$

where $W_k > 0$ is the path size contribution weighting of route $i \in R$ to path size terms (different for each model), so that the contribution of route $k$ to the path size term of route $i$ (the path size contribution factor) is $\frac{W_k}{W_i}$. To dissect the path size term: each link $a$ in route $i$ is penalised (in terms of decreasing the path size term and hence the utility of the route) according to the number of routes in the choice set that also use that link $\left(\sum_{k\in R} \delta_{a,k}\right)$, where each contribution is weighted (i.e. $\sum_{k\in R} \left(\frac{W_k}{W_i}\right) \delta_{a,k}$), and the significance of the penalisation is also weighted according to how prominent link $a$ is in route $i$, i.e. the cost of route $a$ in relation to the total cost of route $i$ $\left(\frac{t_a}{c_i}\right)$.

Path size terms sometimes suppose that the link-route prominence feature is represented as the ratio of link-route length, i.e. $\frac{t_a}{c_i} = \frac{l_a}{L_i}$, where $l_a$ and $L_i$ are the lengths of link $a \in A$ and route $i \in R$, respectively. However, this may be inaccurate in how travellers perceive the prominence of links in a route: a short link may be highly congested and have a greater travel time than a long link that is uncongested, and hence the timely, short link may be perceived as more prominent in the route than the long, quick link. Thus, for internal consistency, we suppose the link-route prominence feature is represented as the ratio of link-route generalised travel cost.

The Path Size Logit (PSL) model (Ben-Akiva & Bierlaire, 1999) proposes that $W_k = 1$ so that all routes contribute equally to path size terms. This is problematic, however, as the correction terms and thus the choice probabilities of realistic routes are affected by link sharing with unrealistic routes. To combat this, Ramming (2002) proposed the Generalised Path Size Logit (GPSL) model where $W_k = c_k^{-\lambda}$ and routes contribute according to travel cost ratios, so that routes with excessively large travel costs have a diminished impact upon the correction terms of routes with small travel costs, and consequently the choice probabilities of those routes. Duncan et al (2020) reformulate the GPSL model (proposing the alternative GPSL model (GPSL$'$)) so that the contribution weighting resembles the probability relation, i.e. $W_k = e^{-\lambda c_k}$. As they discuss, however, GPSL and GPSL$'$ are not internally consistent in how they define routes as being unrealistic: the path size terms consider only travel cost, whereas the route choice probability relation considers disutility *including* the correction term. To address this, the Adaptive Path Size Logit (APSL) model is proposed where $W_k = P_k$ and routes contribute according to ratios of route choice probability. This ensures internal consistency, where routes defined as unrealistic by the path size terms – and consequently given reduced path size contributions – are exactly those with very low choice probabilities. Since the APSL path size contribution factors depend upon the route choice probabilities, the probability relation is an implicit function, naturally expressed as a fixed-point problem. The APSL model is thus not closed-form and solving the choice probabilities requires a fixed-point algorithm to compute the solution. Furthermore, in order to prove existence and uniqueness of solutions the APSL probability relation is modified from that in (1). See Duncan et al (2020) for more details on the derivation and theoretical properties of the APSL model, as well as definitions and details of the other Path Size Logit models.

## 2.3 Bounded Choice Model

In this subsection we briefly formulate the Bounded Choice Model (BCM), see Watling et al (2018) for more details on the derivation and theoretical properties of the model. The BCM proposes that a bound is applied to the difference in random utility between each given alternative and an imaginary reference alternative, so that an alternative only receives a non-zero choice probability if the difference between its random utility and the random utility of the reference alternative is within the bound. Furthermore, the probability each alternative is chosen relates to the odds associated with choosing each alternative versus the reference alternative. Watling et al (2018) consider a special case of the BCM where the reference alternative is the alternative with the maximum deterministic utility. While the application of the BCM can involve exerting an absolute bound upon the difference in utility from the maximum, (for example 25 units worse in deterministic utility), we consider in this paper exerting a relative bound upon the difference, i.e. where routes only receive a non-zero choice probability if they have a deterministic disutility less than $\varphi$ times worse than the greatest route utility. If $V_i < 0$ is the deterministic disutility of alternative $i \in R$, then the probability of alternative $i \in R$ is chosen under the BCM is:

$$P_i = \frac{(h_i(\boldsymbol{V}) - 1)_+}{\sum_{j \in R} \left(h_j(\boldsymbol{V}) - 1\right)_+}, \tag{3}$$

where $h_i(\boldsymbol{V}) = \exp(V_i - \varphi \max(V_k: k \in R))$, $\varphi > 1$ is the relative bound parameter to be estimated, and $(\cdot)_+ = \max(0, \cdot)$. The BCM formulation in (3) is derived from an assumption that the difference random variable error terms (relative to the best alternative) follow a truncated logistic distribution, see Appendix A for details.

In a route choice context where the deterministic utility of route $i \in R$ is given by $V_i = -\theta c_i$, the choice probability relation for route $i \in R$ is:

$$P_i = \frac{(h_i(-\theta \boldsymbol{c}) - 1)_+}{\sum_{j \in R} \left(h_j(-\theta \boldsymbol{c}) - 1\right)_+}, \tag{4}$$

where $h_i(-\theta \boldsymbol{c}) = \exp(-\theta c_i - \varphi \max(-\theta c_l: l \in R)) = \exp\left(-\theta (c_i - \varphi \min(c_l: l \in R))\right)$. Thus, routes only receive a non-zero choice probability if they have a cost less than $\varphi$ times the cost on the cheapest route. We would like to point out that although for simplification of notation $c_i$ is denoted as a single variable, $c_i$ is actually a weighted sum of route variables, i.e. $c_i\left(\boldsymbol{t}(\boldsymbol{w}; \boldsymbol{\alpha})\right) = \sum_{a \in A_i} t_a(\boldsymbol{w}_a; \boldsymbol{\alpha})$, for example travel time, length, number of left/right turns, toll, etc., each with an associated taste coefficient / parameter. Therefore, the bound is applied to generalised cost.

On the surface there may appear to be some similarity between the BCM and the original Random Regret Minimisation (RRM) model (Chorus et al, 2008), in that they both propose that when travellers are considering the relative attractiveness of a route, they compare the route alternative against better alternatives, and worse alternatives in some way (at least in theory) have eliminated effects on better alternatives. For the BCM, the generalised travel cost of a route is compared against that of the lowest costing (best) alternative, and if it has a cost some order of magnitude worse, it is not considered as a realistic alternative and is assigned a zero choice probability. As such, the worse alternatives do not affect the choice probabilities of better alternatives. For the RRM model, however, each of the cost attributes of a route are individually compared against the attributes of the other routes, and if the attribute of another route is worse than the attribute from the route in question, then there is no regret. As such, the worse alternatives do not affect the systematic regrets of better alternatives. Therefore, the BCM and RRM model are very different models. They differ in many ways, but a key difference is that in the RRM model all routes receive non-zero choice probabilities, and thus unrealistic routes in the choice set negatively impact results. Moreover, RRM operates on an attribute level. Prato (2014) explores integrating correction term models with the RRM model, to also deal with route overlap.

# 3 Derivation of the Proposed Bounded Path Size Model Form

## 3.1 The Natural Form

There is a natural form for a Bounded Path Size (BPS) choice model, which is derived as follows. Path Size RUMs (with additive error terms) propose that the deterministic utility for route $i \in R$ is given by $V_i = -\theta c_i + \beta \ln(\gamma_i)$. Thus, inserting the Path Size choice model utilities into the BCM formula in (3), the choice probability relation for route $i \in R$ is:

$$P_i = \frac{(h_i(-\theta \boldsymbol{c} + \beta \ln(\boldsymbol{\gamma})) - 1)_+}{\sum_{j \in R} \big(h_j(-\theta \boldsymbol{c} + \beta \ln(\boldsymbol{\gamma})) - 1\big)_+}, \tag{5}$$

where $h_i(-\theta \boldsymbol{c} + \beta \ln(\boldsymbol{\gamma})) = \exp(-\theta c_i + \beta \ln(\gamma_i) - \varphi \max(-\theta c_l + \beta \ln(\gamma_l) : l \in R))$. So, the natural BPS model form applies a bound to the route utilities so that zero choice probabilities are assigned to routes with infeasibly low utilities ($\varphi$ times worse in utility than the best alternative), where the utilities include a path size correction.

Appropriately defining the path size contribution factors within the path size terms is difficult, however, and from exploring different options, we consequently establish desired properties for a BPS model. We briefly detail and discuss these properties here, see Appendix C for demonstrations on how they are derived. While it may appear the properties are derived from issues with the specific path size term options explored, the natural BPS model form is actually deeply problematic and there are no behaviourally and practically desirable formulations, as we attempt to demonstrate. We define the *active choice set* as the set of routes with non-zero choice probabilities, otherwise known as the used routes or those considered realistic. The Desired Properties (DP) are as follows:

- **Desired Property 1 – Consistent Definitions of Unrealistic Routes:** *Routes defined as unrealistic by the choice model (assigned zero choice probabilities) should have zero path size contributions, and vice versa.*
- **Desired Property 2 – Well-Defined Functions:** *The model functions should be well-defined across their domain.*
- **Desired Property 3 – Internal Consistency:** *The model should be internally consistent, i.e. there is a consistent assessment of the feasibility of routes between probability relation and path size contribution factors.*
- **Desired Property 4 – Uniqueness:** *Route choice probability solutions are inter-active-choice-set unique (where there is only one active choice set in which solutions exist), and conditions can be established for intra-active-choice-set uniqueness (where for a given active choice set there is only one solution).*
- **Desired Property 5 – Continuity:** *The choice probability function is continuous.*

DP1 is behaviourally desirable since otherwise the assumption would be that travellers account for overlap between routes they do not consider as being realistic alternatives, or vice versa in that they do not account for the overlap between some routes they do consider realistic. Achieving this property is not trivial however as it involves zero path size contributions, which results in issues leading to DP2,4,5. DP2 is practically desirable as it allows solutions to exist and be computed, and derives from an issue inherent with the natural BPS model form where zero path size contributions results in occurrences of $\frac{0}{0}$ and $\ln(0)$. DP3 is motivated by the key behavioural feature of the APSL model, where theoretical consistency is provided within the model's specification. We note that internal consistency also includes utilising the same generalised costs within all model components, i.e. also within the path size terms, rather than using just length. Due to inherent $\frac{0}{0}$ and $\ln(0)$ issues with the natural BPS model form, there are problems with solution uniqueness where multiple active choice sets can yield solutions. This is undesirable as then an active choice set selection procedure is required to determine which routes are considered realistic. DP4 is thus that solutions exist within a single active choice only (i.e. so that the choice model has a unique selection of which routes are considered (un)realistic), and that conditions exist for unique solutions within that active choice set (for example conditions exist for unique APSL solutions). DP5 is practically desirable as this property is required for applications of the model, for example parameter estimation and network equilibrium where the costs are not fixed.

We would like to emphasise that continuity of the choice probability function is not trivial for a choice model with implicit restriction of routes (i.e. where zero choice probabilities are assigned). For route choice models in which non-zero choice probabilities are assigned to all routes (i.e. non-bounded models), while the choice probability functions may be continuous for a given choice set, the functions are not continuous for changes to the choice set. As such, as the generalised cost of a route increases where at some point it is excluded by the choice set generation criteria, the probabilities from the choice model will not be continuous. The BCM solves this by ensuring a routes choice probability tends towards zero as its cost increases, and receives a zero probability exactly at the bound (and thus the probabilities of other routes are not adjusted when it is removed from the active choice set). For a BPS model to be continuous, the path size contributions must tend towards zero as a route approaches zero choice probability, and be eliminated exactly at zero choice probability.

DP2,4,5 are general desired properties for any route choice model, and satisfying these properties is essential for application of the model. Often, closed-form models such as MNL, PSL, GPSL, and the BCM satisfy these properties trivially. However, these models have behavioural deficiencies: PSL models do not (fully) deal with unrealistic routes, the BCM does not capture route correlations, and MNL deals with neither route overlap nor unrealistic routes. Our aim is thus to develop a model that can harness the contrasting strengths of the BCM and PSL models, thereby dealing with route overlap *and* unrealistic routes. The difficulty, however, lies in obtaining theoretical consistency, i.e. satisfying DP1&3, where overlap is considered between only and all the routes defined as realistic. While there exist natural BPS model formulations that satisfy DP2,4,5 (e.g. option 1 in Section 10.1.1), and formulations that satisfy DP1&3 (e.g. options 2&3 in Section 10.1.2), no formulations exist where all properties are satisfied.

As shown in Appendix A of the revised manuscript, the BCM is derived from an assumption that the random error terms follow a truncated logistic distribution, where the truncation is dependent upon the bound. For the natural BPS model form in (5), the bound is dependent upon the best route utility, which includes the path size correction. Therefore, during calibration the path size correction can have an indirect effect on both the deterministic utility and random error term. The natural BPS model form could thus in principle correct the relative sizes of the deterministic and random parts of the utility across different routes, and thereby has the potential to provide a means for capturing a greater part of the correlation than standard PSL models, which capture correlations through correcting the deterministic part only (Ramming, 2002; Hoogendoorn-Laser et al, 2005). As shown in Appendix C, however, the natural BPS model form is not suitable for use. In the following section we discuss how this applies to the alternative BPS model form we propose.

## 3.2 The Proposed Form

To circumvent these issues with the natural form for a BPS model, we derive an alternative BPS model form (henceforth just referenced as the proposed BPS model form). In Sections 4&5 we develop two BPS models that adopt the proposed form, and which satisfy desired properties, as we discuss/demonstrate in Appendix E.

The basis for the proposed BPS model form can be considered to roughly derive from the union of two models, where the probability of choosing route $i$ relates to the probability of choosing route $i$ under model 1 and choosing route $i$ under model 2. Model 1 is the BCM and model 2 is a Path Size Logit model where only the correlation between routes is considered, i.e. there is no travel cost component. Let $Q_i^1$ and $Q_i^2$ be the probability of choosing route $i \in R$ under model 1 and model 2, respectively. Unionising the two models, the probability of choosing route $i \in R$ relates as:

$$P_i = Q_i^1 \times Q_i^2 \times \chi,$$

where

$$Q_i^1 = \frac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l : l \in R))\right) - 1\right)_+}{\sum_{j \in R}\left(\exp\left(-\theta\left(c_j - \varphi \min(c_l : l \in R)\right)\right) - 1\right)_+}, \qquad Q_i^2 = \frac{e^{\beta \ln(\gamma_i)}}{\sum_{j \in R} e^{\beta \ln(\gamma_j)}},$$

and $\chi$ is a normalisation constant that ensures the probabilities for all routes sum up to 1. So, $Q_i^1$ is the BCM choice probability relation in (4) and $Q_i^2$ is the regular Path Size Logit model probability relation in (1) with $\theta = 0$, i.e. considering route distinctiveness only. The deterministic utilities of route $i$ under model 1 and model 2 are $V_i^1 = -\theta c_i$ and $V_i^2 = \beta \ln(\gamma_i)$, respectively. By giving both of these utilities i.i.d Gumbel distributed random error terms, the resultant union model would be a regular Path Size Logit model. Instead, model 2 has i.i.d Gumbel distributed random error terms, and model 1 has difference random variable error terms (relative to the best alternative) that follow a truncated logistic distribution (see Appendix A).

With probability relation $P_i = Q_i^1 \times Q_i^2 \times \chi$ and the knowledge that $\sum_{i \in R} P_i = \sum_{i \in R} Q_i^1 \times Q_i^2 \times \chi = 1$, the following BPS model is derived (see Appendix B for details):

$$\begin{aligned} P_i &= \frac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l : l \in R))\right) - 1\right)_+ \cdot e^{\beta \ln(\gamma_i)}}{\sum_{j \in R}\left(\exp\left(-\theta\left(c_j - \varphi \min(c_l : l \in R)\right)\right) - 1\right)_+ \cdot e^{\beta \ln(\gamma_j)}} \\ &= \frac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l : l \in R))\right) - 1\right)_+ \cdot (\gamma_i)^\beta}{\sum_{j \in R}\left(\exp\left(-\theta\left(c_j - \varphi \min(c_l : l \in R)\right)\right) - 1\right)_+ \cdot (\gamma_j)^\beta}. \end{aligned}$$

Note that the proposed BPS model form approaches the regular Path Size Logit model in (1) in the limit as $\varphi \to \infty$ since the BCM approaches the MNL model in limit as $\varphi \to \infty$.

Assuming that the path size terms are non-zero, a route only receives a zero choice probability if $c_i > \varphi \min(c_l: l \in R)$. One can thus predetermine the unused routes by checking the fixed route travel costs against the bound, and the model can be formulated as follows. Let $\bar{R}(\boldsymbol{c}; \varphi) \subseteq R$ be the restricted choice set of all routes $i \in R$ where $c_i < \varphi \min(c_l: l \in R)$. The choice probability relation for route $i \in R$ is:

$$P_i = \begin{cases} \dfrac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot (\gamma_i)^\beta}{\sum_{j \in \bar{R}(\boldsymbol{c};\varphi)} \left(\exp\left(-\theta\left(c_j - \varphi \min(c_l: l \in R)\right)\right) - 1\right) \cdot \left(\gamma_j\right)^\beta} & if\ i \in \bar{R}(\boldsymbol{c}; \varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c}; \varphi) \end{cases}.$$

Routes $i \in \bar{R}(\boldsymbol{c}; \varphi)$ are the used/active routes and routes $i \notin \bar{R}(\boldsymbol{c}; \varphi)$ are the unused/inactive routes.

Proposing that the routes with zero choice probabilities are exactly those with zero path size contributions (and strictly positive otherwise), the BPS model formulation can be extended as follows. Let $\bar{R}(\boldsymbol{c}; \varphi) \subseteq R$ be the restricted choice set of all routes $i \in R$ where $c_i < \varphi \min(c_l: l \in R)$. Given $\bar{R}(\boldsymbol{c}; \varphi)$, the choice probability relation for route $i \in R$ is:

$$P_i = \begin{cases} \dfrac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot (\bar{\gamma}_i)^\beta}{\sum_{j \in \bar{R}(\boldsymbol{c};\varphi)} \left(\exp\left(-\theta\left(c_j - \varphi \min(c_l: l \in R)\right)\right) - 1\right) \cdot \left(\bar{\gamma}_j\right)^\beta} & if\ i \in \bar{R}(\boldsymbol{c}; \varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c}; \varphi) \end{cases}, \tag{6}$$

where the path size term for route $i \in \bar{R}(\boldsymbol{c}; \varphi)$ is:

$$\bar{\gamma}_i = \sum_{a \in A_i} \frac{t_a}{c_i} \frac{W_i}{\sum_{k \in \bar{R}(\boldsymbol{c};\varphi)} W_k \delta_{a,k}}, \tag{7}$$

where $W_i > 0$ is the path size contribution weighting of route $i \in \bar{R}(\boldsymbol{c}; \varphi)$ to used route path size terms, so that the contribution of used route $k$ to the path size term of used route $i$ is $\frac{W_k}{W_i}$. Note that the path size contribution factor is of the form $\frac{W_k}{W_i}$ so that distinct routes non-overlapping with all other routes have path size terms equal to 1. As Ramming (2002) noted, this was an issue for the original alternative PSL formulation proposed by Ben-Akiva & Bierlaire (1999). Since it is predetermined which routes are the unrealistic routes with zero probabilities, one only need consider the correlation between the realistic routes with positive probabilities (i.e. sum over routes $k \in \bar{R}(\boldsymbol{c}; \varphi)$), and inactive/unused routes, i.e. routes $i \notin \bar{R}(\boldsymbol{c}; \varphi)$, do not have path size term values.

For the choice probability function to be continuous for the proposed BPS model, the path size contributions weightings ($W_i$) must tend to zero as the route costs approach the bound from below (and consequently zero choice probability), so that when the cost of a route reaches the bound exactly (and thus receives a zero choice probability and is removed from the active choice set), there are no adjustments to the path size terms of the remaining active routes altering the probabilities and making the distribution discontinuous. This means that the $W_i$ contribution weightings should be explicitly or implicitly dependent upon the route/link costs.

Watling et al (2018) remark that the BCM is consistent with a behavioural assumption that travellers make decisions in two stages. In the context of route choice, in the first stage travellers compare the random utility of each route against the best alternative in a pairwise manner. The bound imposed implicitly generates a choice set. In the second stage, alternatives from this choice set are compared and route choice probabilities are modelled using the log-odds from the first stage. Use of these log-odds means that choice set generation and route choice are consistent with the same underlying behavioural model.

With the natural BPS model form, the deterministic utilities comprise of a path size component and a cost component. This combined utility is used in the first stage to compare and bound, and obtain a choice set. In the second stage, the route choice probabilities are modelled by directly using the log-odds from the first stage.

With the proposed BPS model form derived here, the first stage is identical to that for the standard use of the BCM, where solely travel cost is used to compare and bound to obtain a choice set. Where the proposed BPS model form differs, however, is that in the second stage, the route choice probabilities are not modelled by directly using the log-odds from the first stage, and instead these log-odds are adjusted according to path size corrections to heuristically capture route correlation. Importantly though, the consistent criteria for determining choice sets and route choice probabilities are not violated, i.e. no route excluded from the generated choice set during the first stage can have a non-zero choice probability in the second stage, or vice versa. The key feature of the proposed BPS model form is that the measure of route correlation in the second stage only considers overlap between routes deemed realistic in the first stage.

As discussed in the previous section for the natural BPS model form, since the random error terms depend upon the bound, and the bound in that case is dependent upon the best route utility (which includes the path size correction), during calibration the path size correction can have an indirect effect on both the deterministic utility and random error term. For the proposed BPS model form in (6), however, the bound (in model 1) depends only upon the best route cost and is independent from the path size correction. The path size correction in this case therefore does not affect random error.

## 4 The Bounded Bounded Path Size Model

In this and the following sections, we formulate two BPS models that adopt the proposed form in (6)-(7). In Appendix E we discuss/demonstrate how these two models satisfy the desired properties for a BPS model established in Appendix C.

We begin by formulating the Bounded Bounded Path Size (BBPS) model, which is defined as follows. Let $\bar{R}(\boldsymbol{c};\varphi) \subseteq R$ be the restricted choice set of all active routes $i \in R$ where $c_i < \varphi \min(c_l: l \in R)$. Given $\bar{R}(\boldsymbol{c};\varphi)$, the choice probability relation for route $i \in R$ is:

$$P_i = \begin{cases} \dfrac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot (\bar{\gamma}_i^{BBPS})^{\beta}}{\sum_{j\in\bar{R}(\boldsymbol{c};\varphi)} \left(\exp\left(-\theta\left(c_j - \varphi \min(c_l: l \in R)\right)\right) - 1\right) \cdot \left(\bar{\gamma}_j^{BBPS}\right)^{\beta}} & if\ i \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c};\varphi) \end{cases}, \tag{8}$$

where the path size term for route $i \in \bar{R}(\boldsymbol{c};\varphi)$ is:

$$\bar{\gamma}_i^{BBPS} = \sum_{a\in A_i} \frac{t_a}{c_i} \frac{(h_i(-\lambda\boldsymbol{c}) - 1)}{\sum_{k\in\bar{R}(\boldsymbol{c};\varphi)} (h_k(-\lambda\boldsymbol{c}) - 1)\delta_{a,k}}, \tag{9}$$

where $h_i(-\lambda\boldsymbol{c}) = \exp\left(-\lambda(c_i - \varphi \min(c_l: l \in R))\right)$, and the model parameters are $\theta, \lambda > 0$, $\beta \geq 0$, $\varphi > 1$. $P_i$ in (8) is the BBPS model probability relation for route $i \in R$ which adopts the proposed BPS model form in (6), and $\bar{\gamma}_i^{BBPS}$ in (9) is the BBPS model path size term for route $i \in \bar{R}(\boldsymbol{c};\varphi)$, which adopts the form of (7) with $W_k = h_k(-\lambda\boldsymbol{c}) - 1$.

The rationale behind formulating the BBPS path size contribution weightings as $W_k = h_k(-\lambda\boldsymbol{c}) - 1$ was to satisfy the desired properties for a BPS model. As discussed in the previous section, when deriving a BPS model from the proposed form by stipulating how the path size contribution weightings $W_k$ are formulated, there are requirements for the consequent model to have a continuous choice probability function. To ensure a smooth removal of a route from the active choice set, the weighting $W_k$ for each route $k \in \bar{R}(\boldsymbol{c};\varphi)$ must tend towards zero as the cost of that route tends towards the cost bound from above, i.e. as $c_k \to \varphi \min(c_l: l \in R)$, $c_k > \varphi \min(c_l: l \in R)$, and be eliminated exactly at the bound. The BBPS path size contribution weighting $W_k = h_k(-\lambda\boldsymbol{c}) - 1$ was stipulated as such so to satisfy these requirements. As can be seen, when $\lambda = \theta$, $W_k$ matches the travel cost component in the BBPS model probability relation exactly, and thus choice probabilities and path size contributions tend towards zero concurrently and meet at zero.

An additional path size contribution scaling parameter, $\lambda$, is included, in the spirit of the GPSL and GPSL$'$ models, to allow for the de-coupling of the scale of the model from the path size effect. Larger values of $\lambda$ accentuate the differences in cost with the contribution factors, so that the more expensive routes have more diminished (though still positive) contributions. In the same way that the GPSL$'_{(\lambda=\theta)}$ model is developed, however, one can equate the travel cost scales setting by $\lambda = \theta$ – thus formulating the BBPS$_{(\lambda=\theta)}$ model – to improve internal consistency and reduce the number of model parameters to estimate.

The attraction of the BBPS model is that it has a closed-form choice probability expression and hence route choice probability solutions are guaranteed to exist and be unique. The BBPS model is however not fully internally consistent since the path size contribution factors do not consider route distinctiveness, though consistency is improved by setting $\lambda = \theta$.

Moreover, the BBPS model approaches the GPSL$'$ model as $\varphi \to \infty$:

$$\sum_{a\in A_i} \frac{t_a}{c_i} \frac{(h_i(-\lambda\boldsymbol{c}) - 1)}{\sum_{k\in\bar{R}(\boldsymbol{c};\varphi)} \left(h_j(-\lambda\boldsymbol{c}) - 1\right)\delta_{a,k}} \to \sum_{a\in A_i} \frac{t_a}{c_i} \frac{e^{-\lambda c_i}}{\sum_{k\in R} e^{-\lambda c_k}\delta_{a,k}}$$

and

$$\frac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot (\gamma_i)^{\beta}}{\sum_{j\in\bar{R}(\boldsymbol{c};\varphi)} \left(\exp\left(-\theta(c_i - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot \left(\gamma_j\right)^{\beta}} \to \frac{(\gamma_i)^{\beta} e^{-\theta c_i}}{\sum_{j\in R} \left(\gamma_j\right)^{\beta} e^{-\theta c_j}}$$

$$\text{as } \varphi \to \infty.$$

The BBPS$_{(\lambda=\theta)}$ model is thus equivalent to the GPSL$'_{(\lambda=\theta)}$ model in the limit as $\varphi \to \infty$, and the BBPS model is equivalent to the BCM for $\beta = 0$, which is equivalent to the MNL model in the limit as $\varphi \to \infty$.

## 5 The Bounded Adaptive Path Size Model

The Bounded Adaptive Path Size (BAPS) model adopts the proposed BPS model form derived in Section 3 and proposes that routes contribute to path size terms according choice probability ratios to ensure internal consistency and to provide a continuous choice probability function. The BAPS model route choice probability relation is thus an implicit function, naturally expressed as a fixed-point problem.

In the following two subsections we introduce two variants of the BAPS model. We first introduce in Section 5.1 the standard formulation, which is the straightforward definition. However, the probability domain is not defined on a closed set, forcing difficulties proving the existence and uniqueness of solutions. To circumvent this, we also in Section 5.2 formulate a modified version for which we can prove solution existence and establish uniqueness conditions, and where the standard BAPS formulation can be approximated to an arbitrary precision. We then provide a solution method for the modified BAPS model formulation, prove solution existence, and establish uniqueness conditions.

## 5.1 Standard BAPS Model Formulation

The standard BAPS model formulation ($\text{BAPS}_0$) is defined as follows. Let $\bar{R}(\boldsymbol{c};\varphi) \subseteq R$ be the restricted choice set of all active routes $i \in R$ where $c_i < \varphi \min(c_l: l \in R)$. Given $\bar{R}(\boldsymbol{c};\varphi)$, the $\text{BAPS}_0$ model route choice probabilities, $\boldsymbol{P}^*$, are a solution to the fixed-point problem $\boldsymbol{P} = \boldsymbol{f}(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))$, where $f_i$ for route $i \in R$ is:

$$f_i(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})) = \begin{cases} \dfrac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot \left(\bar{\gamma}_i^{BAPS}(\boldsymbol{P})\right)^\beta}{\sum_{j \in \bar{R}(\boldsymbol{c};\varphi)} \left(\exp\left(-\theta\left(c_j - \varphi \min(c_l: l \in R)\right)\right) - 1\right) \cdot \left(\bar{\gamma}_j^{BAPS}(\boldsymbol{P})\right)^\beta} & if\ i \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c};\varphi) \end{cases}, \tag{10}$$

and the path size term for route $i \in \bar{R}(\boldsymbol{c};\varphi)$ is:

$$\bar{\gamma}_i^{BAPS}(\boldsymbol{P}) = \sum_{a \in A_i} \frac{t_a}{c_i} \frac{P_i}{\sum_{k \in \bar{R}(\boldsymbol{c};\varphi)} P_k \delta_{a,k}} = \sum_{a \in A_i} \frac{t_a}{c_i} \frac{1}{\sum_{k \in \bar{R}(\boldsymbol{c};\varphi)} \left(\frac{P_k}{P_i}\right) \delta_{a,k}}, \qquad \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi))}, \tag{11}$$

$$D^{(\bar{R}(\boldsymbol{c};\varphi))} = \left\{\boldsymbol{P} \in \mathbb{R}_{\geq 0}^N : 0 < P_i \leq 1, \forall i \in \bar{R}(\boldsymbol{c};\varphi), and, 0 \leq P_i \leq 1, \forall i \notin \bar{R}(\boldsymbol{c};\varphi), \sum_{j=1}^N P_j = 1\right\},$$

The model parameters are $\theta > 0$, $\beta \geq 0$, and $\varphi > 1$. $\bar{\gamma}_i^{BAPS}(\boldsymbol{P})$ in (11) is the BAPS model path size term function for route $i \in \bar{R}(\boldsymbol{c};\varphi)$ that is a function involving the choice probabilities of all routes, though in effect only the active routes. $f_i(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))$ in (10) is the $\text{BAPS}_0$ model choice probability function for route $i \in R$ which is a function of the used route path size term functions and hence also the choice probabilities. The choice probability relation for route $i \in R$ is given by $P_i = f_i(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))$, which is an implicit equation involving choice probabilities, and hence the $\text{BAPS}_0$ model route choice probabilities, $\boldsymbol{P}^*$, are a solution such that $P_i^* = f_i(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}^*))$, $\forall i \in R$. For a $\text{BAPS}_0$ model route choice probability solution vector $\boldsymbol{P}^*$, $\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}^*)$ is the BAPS model path size term for route $i \in \bar{R}(\boldsymbol{c};\varphi)$, and unused routes, i.e. routes $i \notin \bar{R}(\boldsymbol{c};\varphi)$, do not have path size term values.

$D^{(\bar{R}(\boldsymbol{c};\varphi))}$ is the domain for the fixed-point function $\boldsymbol{f}$, which is dependent upon the active choice set of routes $\bar{R}(\boldsymbol{c};\varphi)$ (and thus the route costs and bound parameter), and stipulates the feasible set of values for the fixed-point variables, which are in this case probabilities $\boldsymbol{P}$. $D^{(\bar{R}(\boldsymbol{c};\varphi))}$ stipulates that the active routes $i \in \bar{R}(\boldsymbol{c};\varphi)$ with costs below the bound must all have non-zero fixed-point variable values (i.e. $P_i > 0$, $\forall i \in \bar{R}(\boldsymbol{c};\varphi)$) ensuring that occurrences of $\frac{0}{0}$ are avoided in the BAPS model path size term functions $\bar{\gamma}_i^{BAPS}(\boldsymbol{P})$, and thus any solution to the fixed-point system also circumvents the issue. The active routes can however assume any non-zero probability value. $D^{(\bar{R}(\boldsymbol{c};\varphi))}$ then stipulates that the inactive routes $i \notin \bar{R}(\boldsymbol{c};\varphi)$ with costs above the bound can assume any probability value (zero or non-zero), though while the domain of $\boldsymbol{f}$ allows for inactive routes to have non-zero fixed-point variable values, by the definition of $f_i$ in (10), any solution to the fixed-point system will have zero probabilities for all inactive routes. $D^{(\bar{R}(\boldsymbol{c};\varphi))}$ also stipulates that the fixed-point variable values should all sum up to 1, as standard for a probability domain.

As (11) shows, for a choice probability solution $\boldsymbol{P}^*$, the contribution of used route $k$ to the BAPS model path size term of used route $i$ is weighted according to the ratio of choice probabilities between the routes $\left(\frac{P_k^*}{P_i^*}\right)$, and hence as a used route approaches zero choice probability its path size contribution approaches zero, until it is considered unrealistic, where it then receives a zero choice probability and its path size contributions are eliminated completely.

It is our belief that there is a strong theoretical and behavioural basis for the $\text{BAPS}_0$ model, and the model captures the best features of the BCM and APSL model. It appears logical that routes are judged as unrealistic (assigned zero choice probability / have zero path size contributions) if they have an excessively large travel cost, but not necessarily unrealistic if they are very indistinct. Routes are still penalised according to their indistinctiveness and the choice probability / path size contribution of route $i$ decreases as $\bar{\gamma}_i^{BAPS}$ decreases, but routes are not bounded according to indistinctiveness.

The $\text{BAPS}_0$ model approaches the APSL model in the limits as $\tau \to 0$ and $\varphi \to \infty$:

$$G_i\left(g_i(\boldsymbol{\gamma}^{APS}(\boldsymbol{P}))\right) \to g_i(\boldsymbol{\gamma}^{APS}(\boldsymbol{P})) \text{ as } \tau \to 0,$$

and,

$$f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})) \to g_i(\boldsymbol{\gamma}^{APS}(\boldsymbol{P})) \text{ as } \varphi \to \infty.$$

The BAPS$_0$ model is also equivalent to the BCM for $\beta = 0$, which is equivalent to the MNL model in the limit as $\varphi \to \infty$.

The BAPS$_0$ model proposes that the path size terms utilise choice probability ratio path size contribution factors; however, referring to the derivation of the proposed BPS model form in Section 3, the choice probabilities are not the model 2 probabilities ($Q_i^2$), but instead those obtained from the union model. Hence, the BAPS$_0$ model is not a direct union of two separate models and instead the models are interdependent.

The complication for the BAPS$_0$ model to be mathematically well-defined is that it is not in the correct form for standard proofs of solution existence and uniqueness to apply. Standard proofs for existence and uniqueness of fixed-point solutions require the domain of the fixed-point function (in this case $\boldsymbol{f}$) to be a compact convex set. The domain of $\boldsymbol{f}$, $D^{(\bar{R}(\boldsymbol{c};\varphi))}$, however, is not a compact convex set since the fixed-point variable value bounds are not closed for all routes: the lower bound for all active routes $i \in \bar{R}(\boldsymbol{c};\varphi)$ is open where these fixed-point variables cannot assume the bound value (i.e. $P_i \neq 0$). As shown in Appendix C for options 2&3, the path size terms cannot be altered to allow for zero path size contribution weightings without losing continuity of the fixed-point function (which is also required for the proofs), and hence in Section 5.2 below we modify the BAPS model so that it is in the correct form for standard proofs to apply.

## 5.2 Modified BAPS Model Formulation

### 5.2.1 Definition

The modified BAPS model is defined as follows. Let $\bar{R}(\boldsymbol{c};\varphi) \subseteq R$ be the restricted choice set (with size $\bar{N}$) of all routes $i$ where $c_i < \varphi \min(c_l: l \in R)$. The BAPS model route choice probabilities, $\boldsymbol{P}^*$, are a solution to the fixed-point problem $\boldsymbol{P} = \boldsymbol{F}\left(\boldsymbol{f}(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))\right)$, where $F_i$ and $f_i$ for route $i \in R$ are:

$$F_i\left(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))\right) = \begin{cases} \tau + (1 - \bar{N}\tau) \cdot f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})) & if\ i \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c};\varphi) \end{cases}, \tag{12}$$

$$f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})) = \begin{cases} \dfrac{\left(\exp(-\theta(c_i - \varphi \min(c_l: l \in R))) - 1\right) \cdot \left(\bar{\gamma}_i^{BAPS}(\boldsymbol{P})\right)^{\beta}}{\sum_{j \in \bar{R}(\boldsymbol{c};\varphi)} \left(\exp\left(-\theta(c_j - \varphi \min(c_l: l \in R))\right) - 1\right) \cdot \left(\bar{\gamma}_j^{BAPS}(\boldsymbol{P})\right)^{\beta}} & if\ i \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c};\varphi) \end{cases}, \tag{13}$$

and the path size term for route $i \in \bar{R}(\boldsymbol{c};\varphi)$ is:

$$\bar{\gamma}_i^{BAPS}(\boldsymbol{P}) = \sum_{a \in A_i} \frac{t_a}{c_i} \frac{P_i}{\sum_{k \in \bar{R}(\boldsymbol{c};\varphi)} P_k \delta_{a,k}}, \qquad \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}, \tag{14}$$

$$D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)} = \left\{\boldsymbol{P} \in \mathbb{R}_{\geq 0}^{N}: \tau \leq P_i \leq (1 - \bar{N}\tau), \forall i \in \bar{R}(\boldsymbol{c};\varphi), and, 0 \leq P_i \leq (1 - \bar{N}\tau), \forall i \notin \bar{R}(\boldsymbol{c};\varphi), \sum_{j=1}^{N} P_j = 1\right\}.$$

The model parameters are $\theta > 0$, $\beta \geq 0$, $\varphi > 1$, and $0 < \tau \leq \frac{1}{\bar{N}}$, where $\tau$ is the perturbation parameter. (13) and (14) are equivalent to (10) and (11) for the standard BAPS model formulation: $\bar{\gamma}_i^{BAPS}(\boldsymbol{P})$ in (14) is the path size term function for route $i \in \bar{R}(\boldsymbol{c};\varphi)$ that is a function involving the choice probabilities, and $f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))$ in (13) is the unadjusted choice probability function for route $i \in R$ which is a function of the used route path size term functions and hence also the choice probabilities. The choice probability relation for route $i \in R$ is given by $P_i = F_i\left(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))\right)$, which is an implicit equation involving choice probabilities, and hence the BAPS model route choice probabilities, $\boldsymbol{P}^*$, are a solution such that $P_i^* = F_i\left(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}^*))\right)$, $\forall i \in R$. The key difference between this modified formulation and the standard formulation is the adjustment function $F_i$. $F_i\left(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}))\right)$ in (12) is the choice probability adjustment function for route $i \in R$ which adjusts the choice probability function $f_i$ for reasons given below.

Duncan et al (2020) construct a choice probability adjustment function $G_i$ for the APSL model motivated by some desired behaviours and required properties for proving existence and uniqueness. Similar motivations led to the construction of the adjustment function $F_i$ for the BAPS model. The Required Properties (RP) for $F_i$ were as follows:

1. $F_i$ must map into itself.
2. $F_i$ must be continuous for all $\boldsymbol{P}$.
3. $F_i$ must be continuously differentiable with respect to $\boldsymbol{P}$ for all $\boldsymbol{P}$.
4. The domain of $F_i$ must be closed and bounded.
5. The domain of $F_i$ must allow the unused routes to have zero choice probabilities but not the used routes.
6. $F_i$ should be able to approximate $f_i$ to arbitrary precision.
7. The domain of $F_i$ should have a lower bound for used routes that can approximate zero to arbitrary precision.

RP 1-4 are required for existence and uniqueness proofs. RP 5 is required so that the used route path size term function $\bar{\gamma}_i^{BAPS}(\boldsymbol{P})$ in (14) and thus $F_i\left(f_i\left(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ in (12) are defined, i.e. to avoid occurrences of $\frac{0}{0}$. RP 6 is desired as it is not our intention for the choice probabilities acquired from the modified formulation to be different to the choice probabilities from the standard BAPS model formulation (where one would exist), and we wish them to be as close as possible. RP 7 is desired as there should be no intentional bounding of the used route choice probabilities; used routes ideally should be able to assume any non-zero probability, but this must be approximated due to the requirement for the domain to be closed and bounded.

So, the formulation of $F_i$ in (12) and its domain $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ have been constructed to satisfy RP 1-7. In Section 10.2 we prove that RP 1-3 are satisfied. The parameter $\tau$ is introduced, and the domain $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ is such that $P_i \geq \tau$, $\forall i \in \bar{R}(\boldsymbol{c};\varphi)$, and since the choice probabilities for all routes sum up to 1: $P_i \leq (1-(\bar{N}-1)\tau)$, $\forall i \in \bar{R}(\boldsymbol{c};\varphi)$. The domain also stipulates that $0 \leq P_i \leq (1-\bar{N}\tau)$ for all $i \notin \bar{R}(\boldsymbol{c};\varphi)$. RP 4 is thus satisfied as $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ is closed and bounded. $\tau$ is restricted to the range $0 < \tau \leq \frac{1}{\bar{N}}$ and thus RP 5 is satisfied as zero choice probabilities are not in the domain for the used routes, and unused routes can have zero probabilities. As $\tau \to 0$, $F_i \to f_i$ satisfying RP 6 and the lower bound for $P_i$ $\forall i \in \bar{R}(\boldsymbol{c};\varphi)$ in $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ tends towards zero satisfying RP 7.

As is the case for the APSL model, the $\tau$ parameter is not a model parameter that requires estimating, it is simply a mathematical construct that ensures RP 1-7 are satisfied. While the modified BAPS model formulation provides the capability, it is not our intention for this model to purposefully compute different choice probabilities to those obtained from the standard formulation for any given theoretical reason. In fact, we desire the choice probabilities to be as close as possible, and hence we advise that only small values of $\tau$ are used. While bounding the non-zero choice probabilities from below results in a discontinuous choice probability function (since used routes cannot have probabilities between 0 and $\tau$), in practice, the range of computable values is naturally limited by computer precision, and hence choice probabilities are always in effect bounded by the smallest computable positive value. Thus, despite the known discontinuity, <u>in applications we use the modified BAPS model formulation with $\tau$ set as a very small value</u> (as small as feasible for computation). With the APSL model proposed in Duncan et al (2020), no difficulties are experienced in practical applications in their analogous approximation of the desired APSL$_0$ model with the parameter $\tau$, and hence it is also expected that the approximation of the BAPS$_0$ model with the proposed BAPS model here will be similarly non-problematic. For the rest of the paper, i.e. for the demonstrations and estimation work, we use the modified BAPS model formulation with $\tau = 10^{-16}$, unless stated otherwise. In Section 7.3.2.2 we briefly investigate the impact of the $\tau$ parameter upon parameter estimation.

The modified BAPS model formulation approaches the APSL model in the limit as $\varphi \to \infty$:

$$f_i\left(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right) \to g_i\left(\boldsymbol{\gamma}^{APS}(\boldsymbol{P})\right) \text{ as } \varphi \to \infty$$

and,

$$F_i\left(f_i\left(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right) \to G_i\left(g_i\left(\boldsymbol{\gamma}^{APS}(\boldsymbol{P})\right)\right) \text{ as } \varphi \to \infty.$$

Both the standard and modified BAPS model formulations are equivalent to the BCM for $\beta = 0$, which is equivalent to the MNL model in the limit as $\varphi \to \infty$.

BAPS model solutions are guaranteed to exist and are unique under certain conditions. To prove these theoretical properties, we appropriately modify the proofs for existence and uniqueness provided for the APSL model in Duncan et al (2020). We include the proofs in Appendix D. Just as for the APSL model, values of $b > 0$ exist such that BAPS model solutions are unique for $\beta$ in the range $0 \leq \beta \leq b$. Though there are cases where solutions are unique for all $\beta \geq 0$ (for example when there are no overlapping used routes), in most cases there is a maximum value for $b$ ($b_{max}$). $\beta$ in the range $0 \leq \beta \leq b_{max}$ is however only a sufficient condition for unique BAPS model solutions, $\beta_{max}$ is the true maximum value where solutions are unique for $\beta$ in the range $0 \leq \beta \leq \beta_{max}$. In Appendix E we propose a method for estimating $\beta_{max}$ (also adapted from that proposed for the APSL model) and demonstrate estimating the uniqueness conditions for the example network. In Sections 7.3.2.2.3 and 7.4.2.3 we demonstrate estimating the uniqueness conditions for the Sioux Falls simulation experiments and real-life large-scale network, respectively.

### 5.2.2 Solution Method

There are many fixed-point algorithms available for solving the BAPS model fixed-point system $\boldsymbol{P} = \boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$. In the studies in this paper we utilise the simplest fixed-point algorithm available: the Fixed-Point Iteration Method (FPIM) (Isaacson & Keller, 1966). The FPIM is the most basic fixed-point algorithm, and other algorithms aim to accelerate the convergence of the FPIM, though require more complicated computations at each iteration $s$. The FPIM for solving the BAPS model fixed-point system $\boldsymbol{P} = \boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ is formulated as follows:

$$P_i^{(s+1)} = F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}\left(\boldsymbol{P}^{(s)}\right)\right)\right), \qquad s = 0,1,2,\ldots$$

such that

$$\lim_{s\to\infty} P_i^{(s+1)} = \lim_{s\to\infty} F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}\left(\boldsymbol{P}^{(s)}\right)\right)\right) = P_i^*, \qquad \boldsymbol{P}^{(0)} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}, \qquad \forall i \in R.$$

A standard convergence statistic we chose to observe in this study is $\ln\left(\sum_{i\in R}\left|P_i^{(s+1)} - P_i^{(s)}\right|\right)$, and the FPIM is said to have converged sufficiently to a BAPS model choice probability solution if:

$$\ln\left(\sum_{i\in R}\left|P_i^{(s+1)} - P_i^{(s)}\right|\right) < \ln\left(10^{-\xi}\right),$$

where $\xi$ is a predetermined convergence parameter. In Sections 7.3.2.2 & 7.4.1.2 we assess the computational performance of the BAPS model in computing choice probabilities and parameter estimation.

# 6 Theoretical Properties

In this section, we first demonstrate on small example networks the theoretical properties of the proposed BPS models and compare with results from MNL, Path Size Logit models, and the BCM. Then, we discuss how the proposed BPS models satisfy the desired properties established for a BPS model in Section 3.1 and Appendix C, and finally illustrate how the models collapse into one another.

In demonstration 1, we demonstrate whether/how the different models deal with route overlap and unrealistic routes. To do this, we adapt the famous 'loop-hole' network (also known as the red-bus/blue-bus network) presented in Cascetta et al (1996), which is Fig. 1 minus link 1. Example network 1 in Fig. 1 has five routes: Route 1: 1 → 3, Route 2: 1 → 4, Route 3: 2 → 3, Route 4: 2 → 4, Route 5: 5. Routes 3-5 all have a travel cost of 1 while Routes 1&2 have a travel cost of $2.5 - \rho$. Route 5 is distinct while Routes 1-4 are correlated, where the degree of correlation depends on $\rho$. As $\rho \to 1$, Routes 1&2 and Routes 3&4 become highly correlated, and (because links 3&4 become negligible compared to links 1&2) the network is in effect reduced to 3 distinct routes consisting of links 1,2,&5. On-the-other-hand, as $\rho \to 0$, link 2 becomes negligible compared to links 3&4 and Routes 3&4 become non-overlapping routes.

Fig. 2 displays for example network 1 the route choice probabilities for the different models as $\rho$ is varied between 0 and 1, $\theta = \beta = \lambda^{GPS'} = \lambda^{BBPS} = 1$, $\varphi = 2$, $\lambda^{GPS} = 5$. As $\rho$ varies between 0 and 1, the cost of Routes 1&2 decreases from 2.5 to 1.5. Since the minimum costing route is 1, the cost bound is 2. Therefore, for $\rho < 0.5$, Routes 1&2 should be considered unrealistic (given the bound criteria) and hence given zero choice probabilities and excluded from route overlap considerations. As shown for MNL and the BCM, because these models fail to account for any route overlap, and Routes 3-5 all have travel costs of 1 for all $\rho$, these routes have equal choice probabilities for all $\rho$, while the BCM gives zero probabilities to routes considered unrealistic and MNL does not. Routes 3-5 should, however, only have equal choice probabilities at $\rho = 0$ (where these routes are all non-overlapping, equal costing, and Routes 1&2 are considered unrealistic). As $\rho$ is increased from 0 to 0.5, the choice probabilities of Routes 3&4 should be reduced to account for the overlap between the two routes, and as $\rho$ is increased from 0.5 to 1, overlap with Routes 1&2 should also be considered as these become realistic. For PSL, while route overlap is considered, the overlap is considered in a non-discriminatory manner between realistic and unrealistic routes, and therefore Routes 3&4 are penalised for overlapping with Routes 1&2 for $\rho < 0.5$. GPSL, GPSL$'$, and APSL all improve upon this shortcoming of PSL by reducing the penalisation incurred upon Routes 3&4 from Routes 1&2 for $\rho < 0.5$. All routes are given non-zero choice probabilities and path size contributions however, and therefore the effects of the unrealistic routes are not fully dealt with. As the plots for the BBPS & BAPS models show, Routes 1&2 receive zero choice probabilities for $\rho < 0.5$, and Routes 3&4 are not penalised for overlapping with Routes 1&2. For $\rho > 0.5$, Routes 1&2 receive non-zero choice probabilities and Routes 3&4 are penalised for overlapping with Routes 1&2.

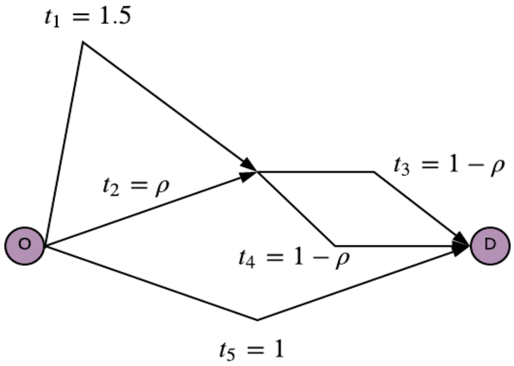



**Fig. 1.** Example network 1.

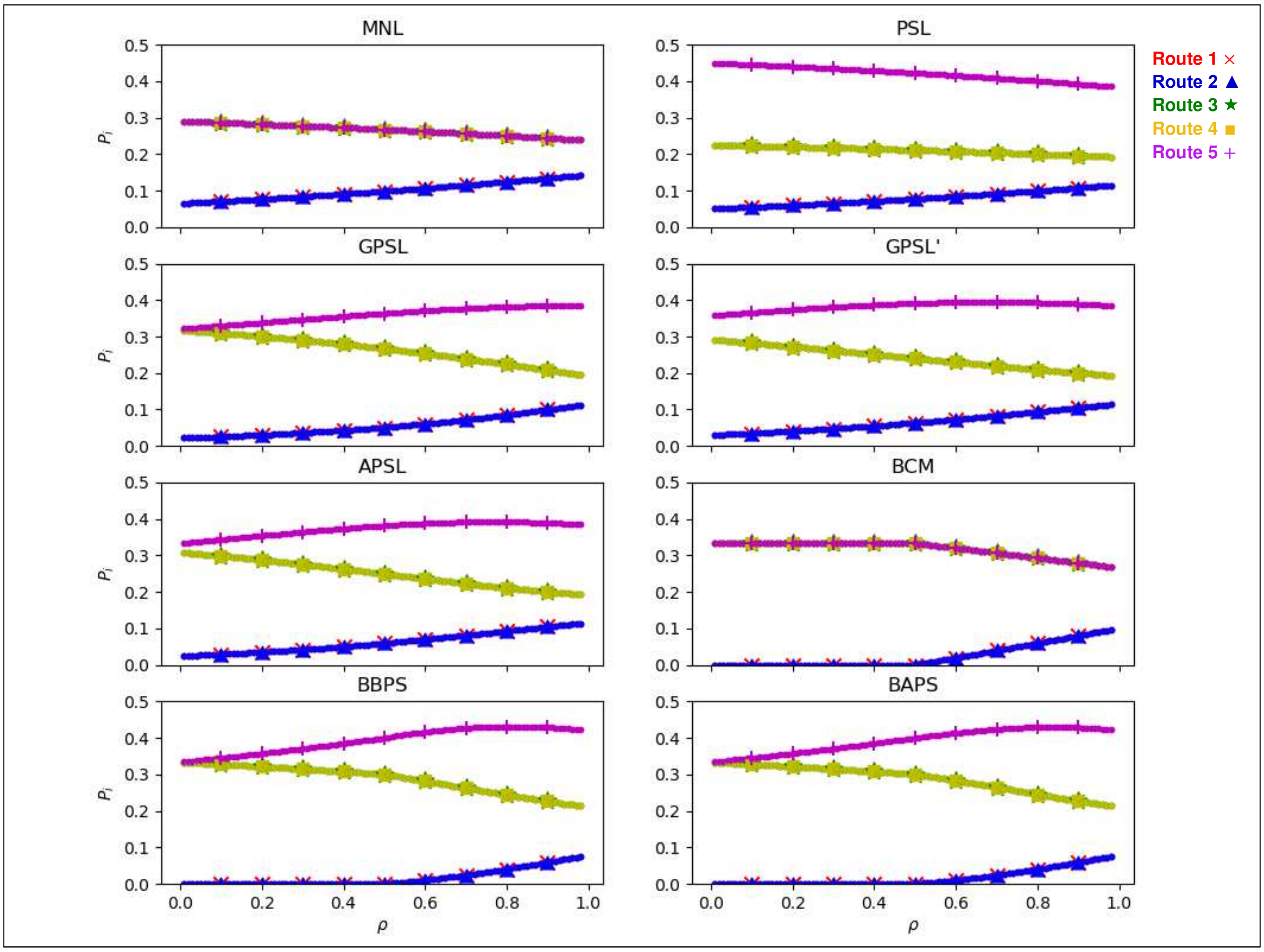



**Fig. 2.** Example network 1: Route choice probabilities for different models as $\rho$ is varied ($\theta = \beta = \lambda^{GPS'} = \lambda^{BBPS} = 1$, $\varphi = 2$, $\lambda^{GPS} = 5$).

In demonstration 2, we demonstrate how the BPS models are able to overcome a drawback typically experienced by correction terms models on the Switching Route Network in Prashker & Bekhor (2004). Example network 2 in Fig. 3 (the Switching Route Network) has four routes: Route 1: 1 → 2. Route 2: 5 → 6. Route 3: 1 → 3 → 6. Route 4: 5 → 4 → 2. Routes 1-3 all have travel cost equal to 10 (for all $\eta$), while Route 4 has travel cost equal $4\eta$-10. To ensure non-negative link costs, $\eta$ must be between 5 and 10. For $\eta = 5$, Route 4 has equal travel cost to the other routes, and as $\eta$ increases from 5, Route 4 increases in cost and consequently becomes less attractive compared to the other routes.

There are expected behaviours from the choice probabilities as $\eta$ is varied between 5 and 10, where the probability of Route 3 is typically observed. For $\eta = 5$, the middle links collapse to zero and the network is in effect reduced to four identical routes. Probability for each of these routes should therefore equal $\frac{1}{4}$ at $\eta = 5$. As $\eta$ increases, Route 4 becomes less attractive and the other routes should increase in choice probability. The proposition is that at some point as $\eta$ is increased, Route 4 should be defined as unrealistic and beyond this point should not impact upon the probabilities of the other routes. Presuming Route 4 is defined as unrealistic before $\eta = 10$, when $\eta$ reaches 10, links 1&6 collapse to zero and the network is in effect reduced to just three identical distinct routes (excluding the unrealistic route). As such, at $\eta = 10$, Route 3 (along with Routes 1&2) should have probability equal to $\frac{1}{3}$. Here, we suppose that a route is defined as unrealistic if it has a travel cost greater than or equal to twice the minimum cost route (a bound of $\varphi = 2$). This means that at and beyond $\eta = 7.5$ (where Route 4's travel cost equals 20), Route 4 should be defined as unrealistic and its impact removed.

Fig. 4A-B displays for example network 2 the Route 3 choice probabilities from the different models as $\eta$ is varied between 5 and 10, where the parameters for Fig. 4A and Fig. 4B are $\theta = \lambda^{GPS'} = \lambda^{BBPS} = \beta = 0.5$, $\varphi = 2$, $\lambda^{GPS} = 10$ and $\theta = \lambda^{GPS'} = \lambda^{BBPS} = 0.1$, $\beta = 0.8$, $\varphi = 2$, $\lambda^{GPS} = 1$, respectively. Considering first Fig. 4A, as shown, for PSL, since the path size terms suppose all routes contribute equally whether realistic or unrealistic, Route 4 contributes to Routes 1&2 for all $\eta$ and the PSL probability for Route 3 goes above $\frac{1}{3}$. For $\eta \geq 7.5$, however, where Route 4 should be defined as unrealistic, Route 4 should not contribute to Routes 1&2. For MNL & the BCM, Routes 1-3 receive the same probability for all $\eta$ as they are equal costing and correlation is not considered. For $\eta \geq 7.5$, the BCM gives the unrealistic Route 4 zero probability (and Route 3 thus $\frac{1}{3}$ probability). MNL gives a non-zero probability, but with the $\theta$ parameter set, these probabilities are small and the BCM is approximated. With the GPSL, GPSL$'$, APSL, BBPS, & BAPS models, overlap correlations between Routes 1-3 are captured, where Route 3 is penalised for overlapping with both Routes 1&2, but because the path size contributions are weighted, the contribution of Route 4 to Routes 1&2 is either reduced (for GPSL, GPSL$'$, APSL) or eliminated (for BBPS & BAPS) for $\eta \geq 7.5$. For the parameters set, GPSL$'$ approximates the BBPS model and APSL approximates the BAPS model, where the contributions are weighted sufficiently for GPSL, GPSL$'$, & APSL such that the probability for Route 3 does not exceed $\frac{1}{3}$.

For the parameters set in Fig. 4B, however, the contributions are not weighted sufficiently for GPSL, GPSL$'$, & APSL, and the probabilities for Route 3 exceed $\frac{1}{3}$. For BBPS & BAPS, with $\varphi = 2$, the contribution of Route 4 to Routes 1&2 will be eliminated for $\eta \geq 7.5$ (rather than reduced) for all settings of the $\theta$ and $\beta$ parameters. $\beta$ allows for route correlations to be captured (differentiating the BPS models from the BCM), while the $\theta$ parameter scales sensitivity to travel cost.

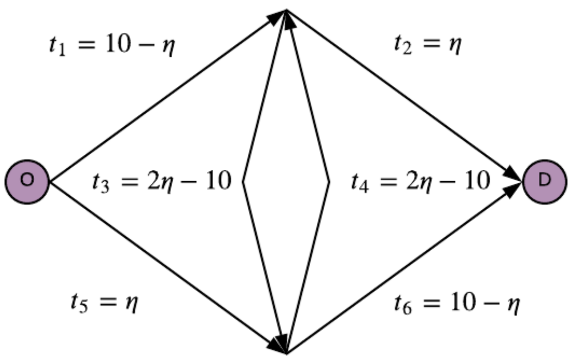



**Fig. 3.** Example network 2 (the Switching Route Network).

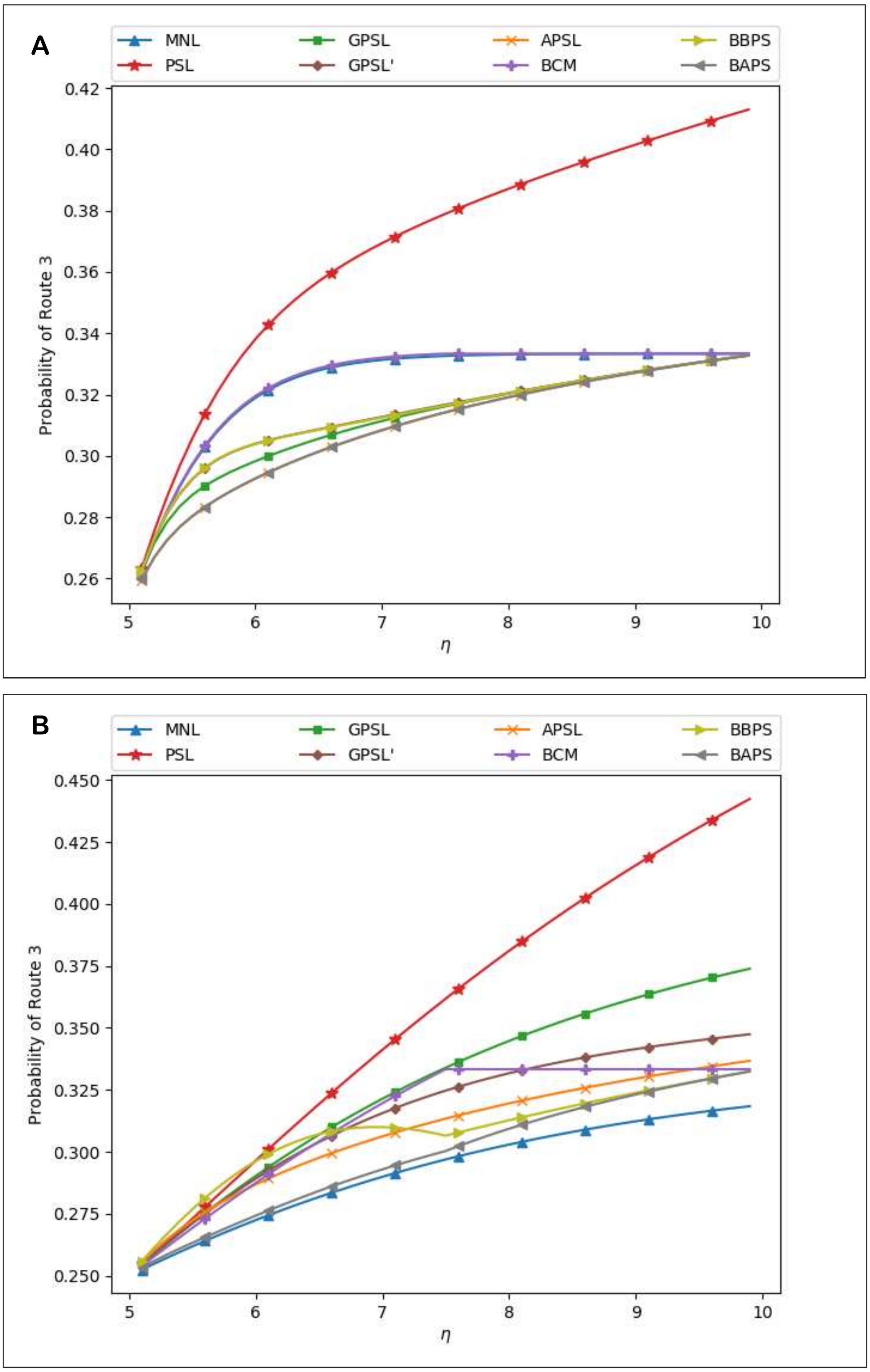



**Fig. 4.** Example network 2: Choice probability of Route 3 for the different models. **A:** $\theta = \lambda^{GPS'} = \lambda^{BBPS} = \beta = 0.5$, $\varphi = 2$, $\lambda^{GPS} = 10$. **B:** $\theta = \lambda^{GPS'} = \lambda^{BBPS} = 0.1$, $\beta = 0.8$, $\varphi = 2$, $\lambda^{GPS} = 1$.

In demonstration 3, we demonstrate how the parameters of the BAPS model impact upon the route choice probabilities. Example network 5 in Fig. 5A has seven routes: Route 1: 1, Route 2: 2, Route 3: 3, Route 4: 4 → 5, Route 5: 4 → 6, Route 6: 7 → 8, Route 7: 7 → 9. Routes 1&7 have travel cost 2, Routes 2&6 have travel cost 1.5, and Routes 3-5 have travel cost 1. Routes 1-3 are distinct routes, while Routes 4&5 and Routes 6&7 are correlated. The minimum costing routes are Routes 3-5 costing 1. For different ranges of the bound parameter $\varphi$, the active choice set of realistic routes varies, and the network can in effect be reduced as follows: for $\varphi > 2$ the full network in Fig. 5A of all 7 seven routes;

for $1.5 < \varphi \leq 2$ the reduced network in Fig. 5B excluding Routes 1&7; and, for $1 < \varphi \leq 1.5$ the reduced network in Fig. 5C excluding Routes 1&7 and Routes 2&6.

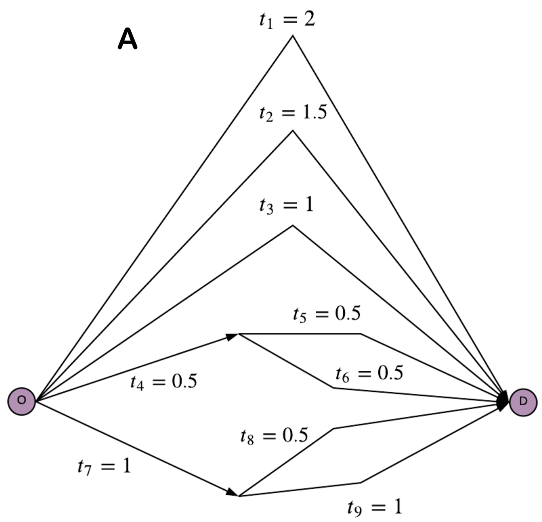
Fig. 6A-E display, for different settings of the $\theta$ and $\beta$ parameters, how the BAPS model choice probabilities vary as $\varphi$ is varied between 1 and 3. Considering first Fig. 6C where $\theta = \beta = 1$, as shown, for $\varphi = 3$, all routes have costs below the bound and thus all have non-zero choice probabilities, (here the APSL probabilities are approximated). As $\varphi$ is decreased to 2, the costs of Routes 1&7 approach the bound, and their choice probabilities thus tend towards zero. Moreover, as Route 7 tends towards zero probability, its path size contribution to Route 6 tends to zero, and thus when $\varphi = 2$ and Route 7 receives zero probability / its contribution to Route 6 is eliminated, the probabilities remain smooth and continuous.

For $\varphi > 2$, despite having the same travel cost, Route 6 has a lower probability than Route 2 as Route 6 is penalised for overlapping with Route 7, while Route 2 is distinct. For $1.5 < \varphi \leq 2$, however, Route 6 is not penalised for overlapping with the unrealistic Route 7, and thus Routes 2&6 have the same probability. As $\varphi$ is decreased to 1.5, Routes 2&6 approach the cost bound and zero probability.

For $1 < \varphi \leq 1.5$, only the minimum costing Routes 3-5 are within the cost bound are thus receive non-zero probabilities. Routes 4&5 have a lower probability than Route 3 since Routes 4&5 are penalised for overlapping.

Now, considering Fig. 5A-C where $\beta$ equals 0, 0.5, and 1, respectively, the effect of the $\beta$ parameter (and thus path size correction) upon route choice can be seen. In Fig. 5A where $\beta = 0$, the BCM probabilities are displayed. As can be seen, Routes 1&7, Routes 2&6, and Routes 3-5 have equal probabilities for all $\varphi$ since these routes have equal costs and route correlation is not considered. Routes 4&5 and Routes 6&7 should be penalised (when considered realistic), however, as they overlap. As Fig. 5B-C show for $\beta = 0.5$ and $\beta = 1$, respectively, the BAPS model probabilities penalises overlapping routes (when they are considered realistic), while the penalisation is more significant for greater values of $\beta$.

Now, considering Fig. 5C-E where $\theta$ equals 1, 0.1, and 2, respectively, the effect of the $\theta$ parameter upon route choice can be seen. Lower $\theta$ values dampen the travel cost differences for routes within the active choice set, and routes with different costs have closer probabilities. Larger $\theta$ values accentuate the travel cost differences so that the higher costing routes receive lower probabilities. Decreasing probabilities with greater $\theta$ values also results in the path size contributions for those routes being reduced, which is why the probabilities between routes with the same cost have closer probabilities for larger $\theta$.



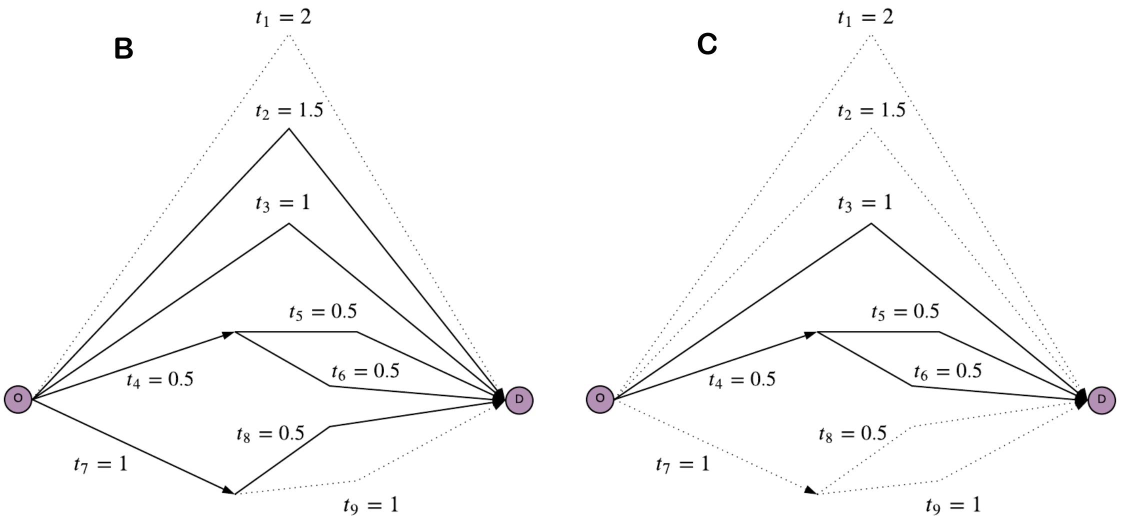
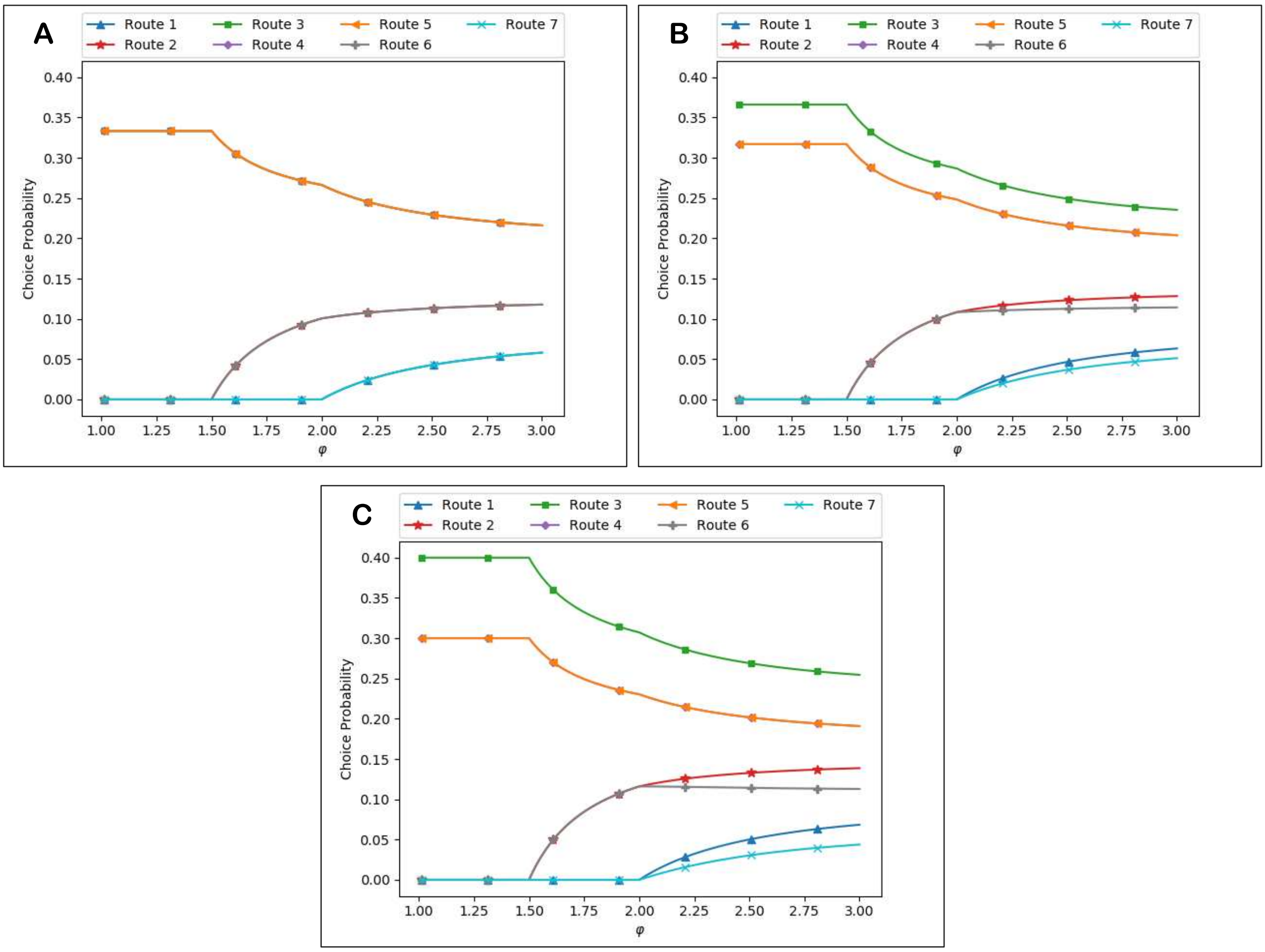



**Fig. 5.** Example network 3. **A:** Full network (for $\varphi > 2$). **B:** Reduced network (for $1.5 < \varphi \leq 2$). **C:** Reduced network (for $1 < \varphi \leq 1.5$).



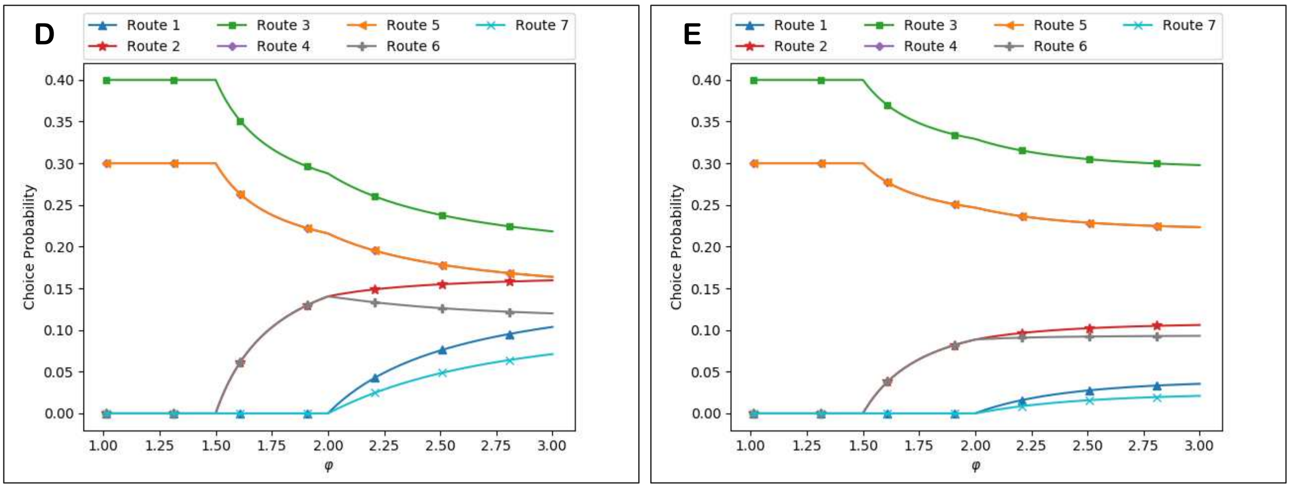



**Fig. 6.** Example network 3: BAPS model choice probabilities as the bound parameter $\varphi$ is varied. **A:** $\theta = 1, \beta = 0$. **B:** $\theta = 1, \beta = 0.5$. **C:** $\theta = \beta = 1$. **D:** $\theta = 0.1, \beta = 1$. **E:** $\theta = 2, \beta = 1$.

Table 1 summarises whether the BBPS, $BAPS_0$, & BAPS models satisfy the established desired properties for a BPS model. We briefly discuss the results below, see Appendix E for a detailed discussion and demonstrations.

Since the BBPS, $BAPS_0$, & BAPS models all adopt the proposed BPS model form as derived in Section 3, DP1 & DP2 are automatically satisfied as the form has a consistent definition for unrealistic routes (which is whether the cost bound is violated) and ensures all functions are defined.

The BBPS model is not internally consistent since route distinctiveness is not considered within the path size contribution factors, while the $BAPS_0$ & BAPS model contribution factors consider choice probability and the models are thus internally consistent. The $BAPS_0$ & BAPS models thus satisfy DP3 while the BBPS model does not.

The BBPS model satisfies DP4 since the BBPS model has a closed-form probability relation guaranteeing solution uniqueness. As discussed in Section 5.1, the $BAPS_0$ model is not in the correct form for standard proofs of solution existence and uniqueness to apply. That is not to say that in all cases solutions are not guaranteed to exist or are not unique, or that it is not the case that solutions do not always exist or there are not always conditions under which solutions are unique. Thus, generally, the $BAPS_0$ model does not satisfy DP4, but this is not necessarily always the case, and is neither proven nor disproven. As proven in Section 10.2, BAPS model solutions are guaranteed to exist and uniqueness conditions can be established, thus satisfying DP4.

The BBPS & $BAPS_0$ model path size contribution weightings tend towards zero as route costs approach the bound from below, and when a route cost reaches the bound exactly, that route receives a zero choice probability / path size contribution. The BBPS & $BAPS_0$ models thus have continuous choice probability functions and hence satisfy DP5. $BAPS_0$ model solutions are not necessarily guaranteed to exist, however, which puts a caveat on whether this is true. The BAPS model does not have a continuous probability function since no route can have a choice probability between 0 and $\tau$, and hence DP5 is not satisfied. The caveat however is that continuity of the BAPS model can be approximated with small values of $\tau$ (the perturbation parameter) such that discontinuity is not an issue in practice.

In conclusion, the benefit of the BBPS model is that solutions are guaranteed to exist and be unique and continuity is guaranteed, while the negative is internal inconsistency. The $BAPS_0$ & BAPS models achieve internal consistency, but the drawbacks are that $BAPS_0$ model solutions are not guaranteed to exist or be unique and the BAPS model choice probability function is not continuous, though both of these drawbacks are not issues in practice. Due to its greater theoretical appeal, and since its lack of discontinuity is not an issue in practice, our recommended is that the BAPS model is used were it is computationally feasible to do so. The BBPS model offers a more computationally practical alternative.

| Desired Property (DP) | BBPS | $BAPS_0$ | BAPS |
|---|---|---|---|
| DP1 – Consistent Definitions of Unrealistic Routes | Yes | Yes | Yes |
| DP2 – Well-Defined Functions | Yes | Yes | Yes |
| DP3 – Internal Consistency | No | Yes | Yes |
| DP4 – Uniqueness | Yes | Neither proven nor disproven | Yes |

| | | | |
|---|---|---|---|
| DP5 – Continuity | Yes | Yes, if solutions exist (neither proven nor disproven) | Yes, in the limit as the 'perturbation parameter' $\tau$ tends to zero |

**Table 1.** Summary of how the BBPS, $\mathrm{BAPS}_0$, & BAPS models satisfy the established desired properties for a BPS model.

Fig. 7 displays a schematic diagram of how the models in this paper collapse into one another.

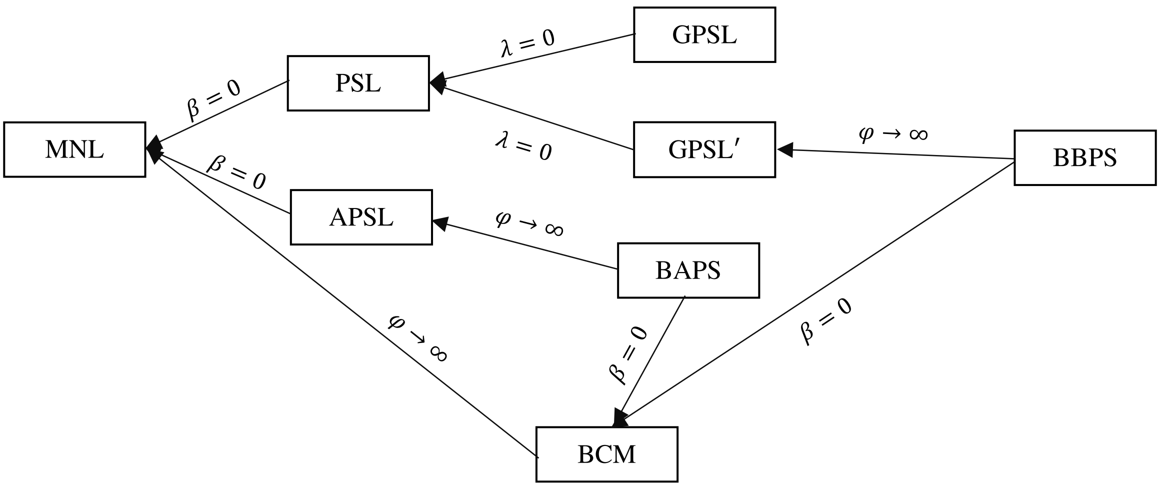



**Fig. 7.** Schematic diagram of how the models collapse into one another.

# 7 Estimating BPS Models

In this section, we provide a Maximum Likelihood Estimation (MLE) procedure for estimating the BBPS & BAPS models with tracked route observations. This procedure is then investigated in simulation studies, and the possibility of reproducing assumed true parameter estimates is assessed. The BBPS & BAPS models are then estimated on a large-scale network using real route choice observation data tracked with GPS units, and results are compared with MNL, Path Size Logit models, and the BCM. As discussed in the Section 5.2.1, in applications, we propose that the modified BAPS model formulation, defined in (12), (13), and (14), is used, with the $\tau$ parameter set as a very small value.

## 7.1 Notation and Definitions for Estimation with Multiple OD Movements

### 7.1.1 Notation

To consider the estimation of the BBPS & BAPS models as well as other models, we extend definitions here for estimation on a network with multiple OD movements, but where the travel costs remain fixed. The road network consists of link set $A$ and $m = 1, \dots, M$ OD movements. $R_m$ is the choice set of all simple routes (no cycles) for OD movement $m$ of size $N_m = |R_m|$, and $A_{m,i} \subseteq A$ is the set of links belonging to route $i \in R_m$, and $\delta_{a,m,i} = \begin{cases} 1 & if\ a \in A_{m,i} \\ 0 & otherwise \end{cases}$. Suppose that the generalised travel cost $t_a$ of each link $a \in A$ is a weighted sum (by parameter vector $\boldsymbol{\alpha}$) of variables $\boldsymbol{w}_a$, i.e. $t_a(\boldsymbol{w}_a; \boldsymbol{\alpha})$, and that the generalised travel cost for route $i \in R_m$, $c_{m,i}$, can be attained through summing up the total cost of its links so that $c_{m,i}\big(\boldsymbol{t}(\boldsymbol{w}; \boldsymbol{\alpha})\big) = \sum_{a \in A_{m,i}} t_a(\boldsymbol{w}_a; \boldsymbol{\alpha})$, where $\boldsymbol{t}$ is the vector of all link travel costs and $\boldsymbol{w}$ is the vector of all link variables. Let the route choice probability for route $i \in R_m$ be $P_{m,i}$, where $\boldsymbol{P}_m = \big(P_{m,1}, P_{m,2}, \dots, P_{m,N_m}\big)$ is the vector of route choice probabilities for OD movement $m$, and $D_m$ is the domain of possible route choice probability vectors for OD movement $m$, $m = 1, \dots, M$.

### 7.1.2 Model Definitions

For multiple OD movement definitions of the MNL, PSL, GPSL, GPSL′, and APSL models for parameter estimation, see Section 5.1.2 in Duncan et al (2020). For the APSL model, the $\tau_m$ parameters are also set here as $\tau_m = 10^{-16}$, $m = 1, \dots, M$, and APSL choice probability solutions are computed using the FPIM with initial conditions set as the MNL route choice probabilities, and convergence statistic set at $\xi = 10$ (see Section 3.4 in Duncan et al (2020)).

We provide here multiple OD movement definitions of the BCM, and the BBPS & BAPS models for parameter estimation.

#### *7.1.2.1 Bounded Choice Model*

The BCM choice probability relation for route $i \in R_m$:

$$P_{m,i}(\boldsymbol{t}) = \frac{\left(\exp\left(-\theta\left(c_{m,i}(\boldsymbol{t}) - \varphi \min\left(c_{m,l}(\boldsymbol{t}): l \in R_m\right)\right)\right) - 1\right)_+}{\sum_{j \in R_m}\left(\exp\left(-\theta\left(c_{m,j}(\boldsymbol{t}) - \varphi \min\left(c_{m,l}(\boldsymbol{t}): l \in R_m\right)\right)\right) - 1\right)_+}. \tag{15}$$

### *7.1.2.2 Bounded Bounded Path Size Model*

Let $\bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \subseteq R_m$ be the restricted choice set (with size $\bar{N}_m$) of all routes $i \in R_m$ where $c_{m,i}(\boldsymbol{t}) < \varphi \min\left(c_{m,l}(\boldsymbol{t}): l \in R_m\right)$ for OD movement $m$. The BBPS choice probability relation for route $i \in R_m$ is:

$$P_{m,i}(\boldsymbol{t}) = \begin{cases} \dfrac{\left(h_{m,i}\left(-\theta \boldsymbol{c}_m(\boldsymbol{t})\right) - 1\right) \cdot \left(\bar{\gamma}_{m,i}^{BBPS}(\boldsymbol{t})\right)^{\beta}}{\sum_{j \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi)}\left(h_{m,j}\left(-\theta \boldsymbol{c}_m(\boldsymbol{t})\right) - 1\right) \cdot \left(\bar{\gamma}_{m,j}^{BBPS}(\boldsymbol{t})\right)^{\beta}} & if\ i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \\ 0 & if\ i \notin \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \end{cases}, \tag{16}$$

where $h_{m,i}\left(-\theta \boldsymbol{c}_m(\boldsymbol{t})\right) = \exp\left(-\theta\left(c_{m,i}(\boldsymbol{t}) - \varphi \min\left(c_{m,l}(\boldsymbol{t}): l \in R_m\right)\right)\right)$, and the path size term for route $i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi)$ is:

$$\bar{\gamma}_{m,i}^{BBPS}(\boldsymbol{t}) = \sum\nolimits_{a \in A_{m,i}} \frac{t_a}{c_{m,i}(\boldsymbol{t})} \frac{\left(h_{m,i}\left(-\lambda \boldsymbol{c}_m(\boldsymbol{t})\right) - 1\right)}{\sum_{k \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi)}\left(h_{m,k}\left(-\lambda \boldsymbol{c}_m(\boldsymbol{t})\right) - 1\right)\delta_{a,m,k}}. \tag{17}$$

### *7.1.2.3 Bounded Adaptive Path Size Model*

Let $\bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \subseteq R_m$ be the restricted choice set (with size $\bar{N}_m$) of all routes $i \in R_m$ where $c_{m,i}(\boldsymbol{t}) < \varphi \min\left(c_{m,l}(\boldsymbol{t}): l \in R_m\right)$ for OD movement $m$. The BAPS model route choice probabilities for OD movement $m$, $\boldsymbol{P}_m^*(\boldsymbol{t})$, are a solution to the fixed-point problem $\boldsymbol{P}_m = \boldsymbol{F}_m\left(\boldsymbol{f}_m\left(\boldsymbol{c}_m(\boldsymbol{t}), \bar{\boldsymbol{\gamma}}_m^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right)\right)$, given the link cost vector $\boldsymbol{t}$, where $F_{m,i}$ and $f_{m,i}$ for route $i \in R_m$ are:

$$F_{m,i}\left(f_{m,i}\left(\boldsymbol{c}_m(\boldsymbol{t}), \bar{\boldsymbol{\gamma}}_m^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right)\right) = \begin{cases} \tau_m + (1 - \bar{N}_m \tau_m) \cdot f_{m,i}\left(\boldsymbol{c}_m(\boldsymbol{t}), \bar{\boldsymbol{\gamma}}_m^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right) & if\ i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \\ 0 & if\ i \notin \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \end{cases}, \tag{18}$$

$$f_{m,i}\left(\boldsymbol{c}_m(\boldsymbol{t}), \bar{\boldsymbol{\gamma}}_m^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right) = \begin{cases} \dfrac{\left(h_{m,i}\left(-\theta \boldsymbol{c}_m(\boldsymbol{t})\right) - 1\right) \cdot \left(\bar{\gamma}_{m,i}^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right)^{\beta}}{\sum_{j \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi)}\left(h_{m,i}\left(-\theta \boldsymbol{c}_m(\boldsymbol{t})\right) - 1\right) \cdot \left(\bar{\gamma}_{m,j}^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right)^{\beta}} & if\ i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \\ 0 & if\ i \notin \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi) \end{cases}, \tag{19}$$

where $h_{m,i}\left(-\theta \boldsymbol{c}_m(\boldsymbol{t})\right) = \exp\left(-\theta\left(c_{m,i}(\boldsymbol{t}) - \varphi \min\left(c_{m,l}(\boldsymbol{t}): l \in R_m\right)\right)\right)$, and the path size term for route $i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi)$ is:

$$\bar{\gamma}_{m,i}^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m) = \sum\nolimits_{a \in A_{m,i}} \frac{t_a}{c_{m,i}(\boldsymbol{t})} \frac{P_{m,i}}{\sum_{k \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi)} P_{m,k}\delta_{a,m,k}}, \qquad \forall \boldsymbol{P}_m \in D_m^{(\bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi))}, \tag{20}$$

$$D_m^{(\bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi),\tau_m)} = \left\{\boldsymbol{P}_m \in \mathbb{R}_{\geq 0}^{N_m}: \tau_m \leq P_{m,i} \leq (1 - (\bar{N}_m - 1)\tau_m), \forall i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi), and, 0 \leq P_{m,i} \leq (1 - \bar{N}_m \tau_m), \forall i \notin \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t}); \varphi), \sum\nolimits_{j=1}^{N_m} P_{m,j} = 1\right\},$$

The model parameters are $\theta > 0$, $\beta \geq 0$, $\varphi > 1$, and $0 < \tau_m \leq \frac{1}{\bar{N}_m}$, $m = 1, \dots, M$. Each OD movement has its own range restrictions for $\tau_m$ based on the number of routes in the active choice set, but the $\tau_m$ parameters are not model parameters that require estimating, and we set $\tau_m = 10^{-16}$, $m = 1, \dots, M$. BAPS model choice probability solutions are computed using the FPIM with initial conditions set as the BCM route choice probabilities, and convergence statistic set at $\xi = 10$ (see Section 5.2.2), unless stated otherwise.

## 7.2 Likelihood Formulations, Existence/Uniqueness, & Estimation Procedure

### 7.2.1 Likelihood Formulations

Suppose that we have available a set of $Z$ observed routes, e.g. collected through GPS units or smart phones, and consider a situation where it is not needed to distinguish individuals in their preferences (the approach is, of course, readily generalised to permit multiple user classes differing in their parameters). Let $m_z$ denote the OD movement of route observation $z$, and for each trip observation $z = 1,2,\dots,Z$, let $R_{m_z}$ be the choice set of all simple routes between the origin and destination of the trip. Suppose that the observation data is contained in a vector $\boldsymbol{x}$ of size $Z$ where:

$$x_z = i \quad \text{if alternative } i \in R_{m_z} \text{ is chosen}, \qquad z = 1,\dots,Z.$$

The BBPS model Likelihood, $L_{BBPS}$, for a sample of size $Z$ is:

$$L_{BBPS}(\boldsymbol{\alpha},\theta,\beta,\varphi,\lambda|\boldsymbol{x}) = \prod_{z=1}^{Z} P_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha});\theta,\beta,\varphi,\lambda), \tag{21}$$

where $P_{m_z,x_z}(\boldsymbol{t})$ is the BBPS model choice probability function given by (16) for route $x_z \in R_{m_z}$.

The BAPS model Likelihood, $L_{BAPS}$, for a sample of size $Z$ is:

$$L_{BAPS}(\boldsymbol{\alpha},\theta,\beta,\varphi|\boldsymbol{x}) = \prod_{z=1}^{Z} P^*_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha});\theta,\beta,\varphi), \tag{22}$$

where $P^*_{m_z,x_z}(\boldsymbol{t})$ is the BAPS model choice probability solution for route $x_z \in R_{m_z}$ to the fixed-point problem $\boldsymbol{P}_{m_z} = \boldsymbol{F}_{m_z}\left(\boldsymbol{f}_{m_z}\left(\boldsymbol{c}_{m_z}(\boldsymbol{t}), \bar{\boldsymbol{\gamma}}^{BAPS}_{m_z}(\boldsymbol{t},\boldsymbol{P}_{m_z})\right)\right)$ for OD movement $m_z$, given the link cost vector $\boldsymbol{t}$, where $F_{m,i}$ and $f_{m,i}$ are as in (18) and (19), respectively, for route $i \in R_m$, and $\bar{\gamma}^{BAPS}_{m,i}$ is as in (20) for route $i \in \bar{R}_m(\boldsymbol{c}_m(\boldsymbol{t});\varphi)$.

If for a given setting of the travel cost and bound parameters $\tilde{\boldsymbol{\alpha}}$ and $\tilde{\varphi}$, there is an observation $z$ such that $c_{m_z,x_z}\left(\boldsymbol{t}(\boldsymbol{w};\tilde{\boldsymbol{\alpha}})\right) \geq \tilde{\varphi}\min\left(c_{m_z,l}\left(\boldsymbol{t}(\boldsymbol{w};\tilde{\boldsymbol{\alpha}})\right): l \in R_{m_z}\right)$, the BBPS & BAPS model Likelihood values are zero. This means that the maximum likelihood estimates $(\hat{\boldsymbol{\alpha}},\hat{\theta},\hat{\beta},\hat{\varphi},\hat{\lambda})$ for the BBPS model and $(\hat{\boldsymbol{\alpha}},\hat{\theta},\hat{\beta},\hat{\varphi})$ for the BAPS model will always be such that $c_{m_z,x_z}\left(\boldsymbol{t}(\boldsymbol{w};\hat{\boldsymbol{\alpha}})\right) < \hat{\varphi}\min\left(c_{m_z,l}\left(\boldsymbol{t}(\boldsymbol{w};\hat{\boldsymbol{\alpha}})\right): l \in R_{m_z}\right)$ for $z = 1,\dots,Z$.

The BBPS model Log-Likelihood function, $LL_{BBPS}$, to be maximised is:

$$LL_{BBPS}(\boldsymbol{\alpha},\theta,\beta,\varphi,\lambda|\boldsymbol{x}) = \ln\left(\prod_{z=1}^{Z} P_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha});\theta,\beta,\varphi,\lambda)\right) = \sum_{z=1}^{Z} \ln\left(P_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha});\theta,\beta,\varphi,\lambda)\right), \tag{23}$$

$$\textit{subject to} \quad c_{m_z,x_z}\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})\right) < \varphi\min\left(c_{m_z,l}\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})\right): l \in R_{m_z}\right), \qquad z = 1,\dots,Z,$$

where $P_{m_z,x_z}(\boldsymbol{t})$ is the BBPS model choice probability relation in (16) for route $x_z \in R_{m_z}$.

The BAPS model Log-Likelihood function, $LL_{BAPS}$, to be maximised is:

$$LL_{BAPS}(\boldsymbol{\alpha},\theta,\beta,\varphi|\boldsymbol{x}) = \ln\left(\prod_{z=1}^{Z} P^*_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha});\theta,\beta,\varphi)\right) = \sum_{z=1}^{Z} \ln\left(P^*_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha});\theta,\beta,\varphi)\right), \tag{24}$$

$$\textit{subject to} \quad c_{m_z,x_z}\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})\right) < \varphi\min\left(c_{m_z,l}\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})\right): l \in R_{m_z}\right), \qquad z = 1,\dots,Z,$$

where $P^*_{m_z,x_z}(\boldsymbol{t})$ is the BAPS model choice probability solution for route $x_z \in R_{m_z}$ to the fixed-point problem $\boldsymbol{P}_{m_z} = \boldsymbol{F}_{m_z}\left(\boldsymbol{f}_{m_z}\left(\boldsymbol{c}_{m_z}(\boldsymbol{t}), \bar{\boldsymbol{\gamma}}^{BAPS}_{m_z}(\boldsymbol{t},\boldsymbol{P}_{m_z})\right)\right)$ for OD movement $m_z$, given the link cost vector $\boldsymbol{t}$.

### 7.2.2 Existence & Uniqueness of Solutions

The typical sufficient conditions for the *existence* of Maximum Likelihood Estimation (MLE) solutions are that: a) the parameter space is compact (closed and bounded), and b) the Likelihood function is a continuous function.

Consider first the BBPS model. Since the BBPS probability function in (16)-(17) is a continuous closed-form function, the BBPS Likelihood function in (21) is in turn also continuous. The range restrictions for the model parameters are $\theta > 0$, $\beta \geq 0$, $\varphi > 1$, $\lambda > 0$, and the travel cost parameters $\boldsymbol{\alpha}$ may have e.g. positive, negative, or no restrictions. Define $\Omega_{BBPS}$ as the parameter space obtained from these range restrictions. $\Omega_{BBPS}$ is not a compact set and thus for this general parameter space the typical sufficient conditions do not apply. This is the same for estimating MNL, PSL, etc, . In practice however it is commonplace to enforce some sensible bounds upon the parameter ranges. Define then $\Omega'_{BBPS} \subseteq \Omega_{BBPS}$ as a closed-bounded parameter subspace of $\Omega_{BBPS}$. For any $\Omega'_{BBPS}$, since the BBPS Likelihood function is continuous, the typical sufficient conditions can be applied, and solutions are guaranteed to exist.

The BBPS Likelihood function in (21) can be rewritten as follows:

$$L_{BBPS}(\boldsymbol{\alpha}, \theta, \beta, \varphi, \lambda | \boldsymbol{x}) = \prod_{z=1}^{Z} \begin{cases} 0 & if\ c_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})) \geq \varphi \min(c_{m_z,l}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})): l \in R_{m_z})\ for\ any\ z \\ P_{m_z,x_z}(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha}); \theta, \beta, \varphi, \lambda) & otherwise \end{cases} \quad (25)$$

For a closed-bounded parameter space $\Omega'_{BBPS} \subseteq \Omega_{BBPS}$, there are three scenarios:

i) For *all* $(\tilde{\boldsymbol{\alpha}}, \tilde{\theta}, \tilde{\beta}, \tilde{\varphi}, \tilde{\lambda}) \in \Omega'_{BBPS}$ the observed routes have travel costs greater than the bound and the Likelihood $L_{BBPS}$ is zero.

ii) For *some* $(\tilde{\boldsymbol{\alpha}}, \tilde{\theta}, \tilde{\beta}, \tilde{\varphi}, \tilde{\lambda}) \in \Omega'_{BBPS}$ the observed routes have travel costs greater than the bound and the Likelihood $L_{BBPS}$ is zero.

iii) For *no* $(\tilde{\boldsymbol{\alpha}}, \tilde{\theta}, \tilde{\beta}, \tilde{\varphi}, \tilde{\lambda}) \in \Omega'_{BBPS}$ the observed routes have travel costs greater than the bound and the Likelihood $L_{BBPS}$ is zero.

Obviously, parameter spaces resulting in i) are not suitable; however, i) occurs only when the upper limit for the bound parameter $\tilde{\varphi}$ is set too low. For any closed-bounded range for the travel cost parameters $\tilde{\boldsymbol{\alpha}}$, upper limits for $\tilde{\varphi}$ will exist such that $\Omega'_{BBPS}$ is either ii) or iii) (since it is always possible to expand the bound $\varphi$ to include at least one observed route). Suppose then that the upper limit for $\tilde{\varphi}$ is set suitably high to avoid i), and we now have case ii). Define $\bar{\Omega}'_{BBPS}$ as the parameter subspace of $\Omega'_{BBPS}$ where no observed routes have travel costs greater than the bound. Since if a MLE solution is to exist, it will exist within the parameter subspace $\bar{\Omega}'_{BBPS}$, and solutions are guaranteed to exist, solutions are guaranteed to exist in $\bar{\Omega}'_{BBPS}$. For case iii), $\bar{\Omega}'_{BBPS} = \Omega'_{BBPS}$ and MLE solutions will exist and can exist in the whole closed-bounded parameter subspace.

For the BAPS model, the BAPS probability function in (18)-(20) is not technically continuous, and thus the BAPS Likelihood function in (22) is not continuous. Existence of MLE solutions thus cannot be guaranteed for the BAPS model. Nevertheless, as discussed in Sections 5.2&6, continuity of the BAPS probability function is not an issue in practice, since continuity can be approximated to arbitrary precision with the $\tau$ parameter. It is therefore believed that the BAPS Log-Likelihood function can also be continuous in practice, and indeed this appeared to be the case in our numerical experiments. When MLE solutions exist, they will exist in $\bar{\Omega}'_{BAPS}$ if case ii) above or in $\bar{\Omega}'_{BAPS} = \Omega'_{BAPS}$ if case iii) above.

The typical sufficient conditions for the uniqueness of MLE solutions are that, given an MLE solution exists: a) the parameter space is convex, and b) the Likelihood function is a concave function. The issue here for the BPS models, is that the probability functions are not guaranteed to be monotonic functions, and thus the Likelihood function is not guaranteed to be concave. This is not to say however that MLE solutions for the BPS models cannot be unique, since these are only sufficient conditions, and no issues with uniqueness were experienced in the experiments in this paper.

### 7.2.3 Estimation Procedure

Standard MLE procedures can be used to estimate the parameters of the BBPS & BAPS models for a given network. Using a standard iterative estimation procedure, BBPS & BAPS model parameters can be found that maximise the Log-Likelihood functions as formulated in (23) and (24) above for a given set of data. Duncan et al (2020) outline algorithm pseudo-code for a tracked route observation data estimation procedure for the APSL model. Using a similar approach, Algorithm 1 below outlines pseudo-code for the BBPS & BAPS model estimation procedure.

Maximising Log-Likelihood for the BPS models is complicated by the constraints that require all chosen routes to have costs less than the cost bound, otherwise the Log-Likelihood functions are undefined. It is possible to pre-determine the parameter space $\bar{\Omega}'$ for MLE (where there Log-Likelihood will always be defined), by identifying (for a given closed-bounded range for the cost parameters) the lower limit for the bound parameter $\varphi$ before it is possible for any chosen route to violate the cost bound. Or, one can incorporate corresponding constraints for the optimisation algorithm, like those in (23) and (24) but adjusted to include equivalence. However, since identifying the existence parameter space / incorporating the corresponding constraints is not always straightforward, we detail in Algorithm 1 and adopt in our experiments an easier to implement approach.

**Step 1: Initialisation.** For each route observation $z = 1, \dots, Z$, generate the corresponding universal choice set and store the link attributes and link-route information. Define an initial set of parameter values $(\tilde{\boldsymbol{\alpha}}^{(1)}, \tilde{\theta}^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)}, \tilde{\lambda}^{(1)})$ for the BBPS model or $(\tilde{\boldsymbol{\alpha}}^{(1)}, \tilde{\theta}^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)})$ for the BAPS model for MLE, and set $n = 1$.

**Step 2: Bound violation check.** Given the travel cost parameters $\tilde{\boldsymbol{\alpha}}^{(n)}$ for iteration $n$, calculate the link costs $\boldsymbol{t}(\boldsymbol{w}; \tilde{\boldsymbol{\alpha}}^{(n)})$ and consequently the route costs $\boldsymbol{c}_{m_z}\left(\boldsymbol{t}(\boldsymbol{w}; \tilde{\boldsymbol{\alpha}}^{(n)})\right)$, $z = 1, \dots, Z$, for iteration $n$. Given the route costs, and the bound parameter value $\tilde{\varphi}^{(n)}$ for iteration $n$, check whether $c_{m_z,x_z}\left(\boldsymbol{t}(\boldsymbol{w};\tilde{\boldsymbol{\alpha}}^{(n)})\right) \geq \tilde{\varphi}^{(n)} \min\left(c_{m_z,l}\left(\boldsymbol{t}(\boldsymbol{w};\tilde{\boldsymbol{\alpha}}^{(n)})\right): l \in R_{m_z}\right)$ for any $z$. If so, set the Log-Likelihood value $LL_{BBPS}^{(n)}$ or $LL_{BAPS}^{(n)}$ for iteration $n$ as an appropriate large and negative value (since $\ln(0)$ is undefined), and skip to Step 4. Otherwise, continue to Step 3.

**Step 3: Recalculate choice probabilities and LL.**

BBPS Model: Given the set of parameter values $\left(\tilde{\boldsymbol{\alpha}}^{(n)}, \tilde{\theta}^{(n)}, \tilde{\beta}^{(n)}, \tilde{\varphi}^{(n)}, \tilde{\lambda}^{(n)}\right)$ and the link and route costs for iteration $n$, compute the BBPS model choice probabilities $P_{m_z,x_z}$ according to (16) and (17) above for $z = 1, \ldots, Z$. Given these probabilities, calculate the BBPS model Log-Likelihood $LL_{BBPS}^{(n)}\left(\tilde{\boldsymbol{\alpha}}^{(n)}, \tilde{\theta}^{(n)}, \tilde{\beta}^{(n)}, \tilde{\varphi}^{(n)}, \tilde{\lambda}^{(1)} \middle| \boldsymbol{x}\right)$ for iteration $n$.

BAPS Model: Given the set of parameter values $\left(\tilde{\boldsymbol{\alpha}}^{(n)}, \tilde{\theta}^{(n)}, \tilde{\beta}^{(n)}, \tilde{\varphi}^{(n)}\right)$ and the link and route costs for iteration $n$, solve each of the fixed-point problems

$$\boldsymbol{P}_{m_z} = \boldsymbol{f}_{m_z}\left(\boldsymbol{c}_{m_z}\left(\boldsymbol{t}(\boldsymbol{w};\tilde{\boldsymbol{\alpha}}^{(n)})\right), \overline{\boldsymbol{\gamma}}_{m_z}^{BAPS}\left(\boldsymbol{t}(\boldsymbol{w};\tilde{\boldsymbol{\alpha}}^{(n)}), \boldsymbol{P}_{m_z}\right); \tilde{\theta}^{(n)}, \tilde{\beta}^{(n)}, \tilde{\varphi}^{(n)}\right)$$

for $z = 1, \ldots, Z$. Given the fixed-point choice probability solutions $P_{m_z,x_z}^{*}$ for each of the route observations $z = 1, \ldots, Z$, calculate the BAPS model Log-Likelihood $LL_{BAPS}^{(n)}\left(\tilde{\boldsymbol{\alpha}}^{(n)}, \tilde{\theta}^{(n)}, \tilde{\beta}^{(n)}, \tilde{\varphi}^{(n)} \middle| \boldsymbol{x}\right)$ for iteration $n$.

**Step 4: Compute new set of parameters.**

BBPS Model: Based on $LL_{BBPS}^{(s)}$ and the associated parameters $\left(\tilde{\boldsymbol{\alpha}}^{(s)}, \tilde{\theta}^{(s)}, \tilde{\beta}^{(s)}, \tilde{\varphi}^{(s)}, \tilde{\lambda}^{(s)}\right)$ for all $s \leq n$, compute a new set of parameters $\left(\tilde{\boldsymbol{\alpha}}^{(n+1)}, \tilde{\theta}^{(n+1)}, \tilde{\beta}^{(n+1)}, \tilde{\varphi}^{(n+1)}, \tilde{\lambda}^{(n+1)}\right)$ to test in the following iteration.

BAPS Model: Based on $LL_{BAPS}^{(s)}$ and the associated parameters $\left(\tilde{\boldsymbol{\alpha}}^{(s)}, \tilde{\theta}^{(s)}, \tilde{\beta}^{(s)}, \tilde{\varphi}^{(s)}\right)$ for all $s \leq n$, compute a new set of parameters $\left(\tilde{\boldsymbol{\alpha}}^{(n+1)}, \tilde{\theta}^{(n+1)}, \tilde{\beta}^{(n+1)}, \tilde{\varphi}^{(n+1)}\right)$ to test in the following iteration.

**Step 5: Stopping criteria.** If $\left|LL_{BBPS}^{(n)} - LL_{BBPS}^{(n-1)}\right| < \zeta$ or $\left|LL_{BAPS}^{(n)} - LL_{BAPS}^{(n-1)}\right| < \zeta$ stop. Otherwise, set $n = n + 1$ and return to Step 2.

**Algorithm 1:** Pseudo-code for estimating the BBPS and BAPS models.

As discussed in Section 7.2.2 above, for a closed-bounded parameter space $\Omega'$ where for some settings of the parameters the Likelihood is zero, the MLE solution will always lie in the parameter subspace $\overline{\Omega}'$ where no observed routes have travel costs greater than the bound and the Likelihood is non-zero. Thus, the idea for Algorithm 1 is simply to tell the algorithm to search for solutions within $\overline{\Omega}'$ only, by setting nonoptimal values for the objective function when testing parameters not in $\overline{\Omega}'$.

To do this, in Algorithm 1 we include a bound violation check in Step 2. In this step, given the route travel costs from the current cost parameters $\tilde{\boldsymbol{\alpha}}^{(n)}$ and the current bound parameter $\tilde{\varphi}^{(n)}$, a check is performed to see whether any chosen route currently violates the cost bound. If any chosen route does violate the bound, then an appropriate large and negative value is set for the Log-Likelihood value. For the experiments in this paper, supposing that $Z'$ is the set of observations that violate the bound, we set the appropriate large and negative value as

$$LL = \sum_{z=1}^{Z} \begin{cases} -999 & if\ z \in Z' \\ \ln\left(P_{m_z,x_z}^{BCM}\right) & otherwise' \end{cases}$$

where $P_{m_z,x_z}^{BCM}$ is the BCM choice probability for route $x_z \in R_{m_z}$ given the current $\tilde{\boldsymbol{\alpha}}^{(n)}$ and $\tilde{\varphi}^{(n)}$ parameter values. Setting the appropriate large and negative value in this way, rather than as some constant arbitrary number, means that some information can be gathered on the relevance of the parameters even when bound violating parameters are tested. For more accurate information, the BBPS or BAPS probabilities can be used instead of the BCM probabilities. We use the BCM probabilities however to avoid having to compute BAPS model fixed-point probabilities for non-relevant parameter tests, thereby reducing computation times.

In general, Step 4 could apply procedures from standard numerical optimisation methods to identify the parameters to evaluate in the next iteration. For cases where there is a single variable in the generalised link travel cost function (for example in the Sioux Falls simulation experiments in Section 7.3.2 below), it is possible to adopt gradient approaches such as Newton-Raphson or BHHH. In this case, the singular cost parameter can be factored out from the cost functions, so that the minimum cost route is fixed (e.g. the route with the quickest free-flow travel time). The min operator component within the bounded model probability functions (see e.g. equations (15), (16), and (19)) can thus be treated as a constant and is independent from any parameters. Therefore, in this case, in the parameter space $\overline{\Omega}'$, the Log-Likelihood objective function is continuously differentiable with respect to the parameters, and gradient minimisation algorithms can be adopted.

For cases where there are multiple variables in the generalised link travel cost function (for example in the real-life case study in Section 7.4 below), however, it is not guaranteed that gradient minimisation algorithms can be directly adopted, since in this case, the minimum cost routes are not guaranteed to be fixed for every OD movement. If for all values of the cost parameters in the stipulated cost parameter space and for all OD movements the minimum cost routes are always the same routes, then the Log-Likelihood objective function is continuously differentiable in the parameter space $\bar{\Omega}'$. It is possible that one could potentially stipulate a cost parameter space to ensure as such. Alternatively, one could smooth out the min operator, at the kinks or by adopting a logsum operator to approximate the min function.

For the BAPS model, however, regardless of whether or not the Log-Likelihood function is continuously differentiable, utilising gradient approaches is complicated by the difficulties in differentiating the BAPS model Log-Likelihood function, which involves differentiating the fixed-point choice probabilities with respect to the parameters, which is not straightforward. Other optimisation algorithms such as BFGS and alternative quasi-Newton algorithms use finite difference to approximate the differentials, and while are more computationally burdensome and typically less accurate, are readily useable. Thus, for the experiments in this paper, we estimate the BBPS and BAPS models utilising the L-BFGS-B bound-constraint, quasi-Newton minimisation algorithm (Byrd et al, 1995) for Steps 2-4 of Algorithm 1 (where we minimise $-LL$). The L-BFGS-B algorithm was implemented using the scipy.optimize.minimize package in Python. The parameter bounds and initial conditions are given in each study.

In Fig. 12 and Fig. 23, we demonstrate how the adopted L-BFGS-B algorithm converges to the parameter estimates for the BAPS model, given the initial conditions. Other initial conditions were tested to see whether different solutions would be found but the solution was the same. Although it is not necessarily a requirement, our recommendation is that initial conditions are set such that none of the chosen route cost bounds are violated, i.e. $\left(\widetilde{\boldsymbol{\alpha}}^{(1)}, \tilde{\theta}^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)}, \tilde{\lambda}^{(1)}\right) \in \bar{\Omega}'_{BBPS}$ or $\left(\widetilde{\boldsymbol{\alpha}}^{(1)}, \tilde{\theta}^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)}\right) \in \bar{\Omega}'_{BAPS}$. This can be done simply by setting an intuitively large bound value, or by calculating $B\left(\widetilde{\boldsymbol{\alpha}}^{(1)}\right) = \max\left(\frac{c_{m_z,x_z}\left(\boldsymbol{t}(\boldsymbol{w};\widetilde{\boldsymbol{\alpha}}^{(1)})\right)}{\min\left(c_{m_z,l}\left(\boldsymbol{t}(\boldsymbol{w};\widetilde{\boldsymbol{\alpha}}^{(1)})\right): l \in R_{m_z}\right)} : z = 1, \dots, Z\right)$ (the lower limit for $\varphi$ before any chosen route violates the bound) given the initial conditions for the cost parameters $\widetilde{\boldsymbol{\alpha}}^{(1)}$, and choosing a larger value than $B\left(\widetilde{\boldsymbol{\alpha}}^{(1)}\right)$.

Note that Algorithm 1 computes one set of parameter estimates, estimated from one set of observations. It is not possible to calculate standard errors for the estimates analytically for the BBPS or BAPS model. This is because the models violate the regularity conditions that establish asymptotic standard errors of the Maximum Likelihood Estimates as the inverse of the Fisher information. Instead, the robustness of the parameters estimated (variation of the estimates) can be investigated numerically by applying Algorithm 1 multiple times through resampling-approaches such as Bootstrap or Jackknife.

## 7.3 Simulation Studies

In this section we investigate the formulated Likelihood functions for the BBPS & BAPS models in simulation studies, evaluating the Likelihood-surfaces and assessing the possibility of estimating reasonable parameters that reproduces observed behaviour.

### 7.3.1 Experiment Setup

A similar approach is adopted to that utilised for the APSL model in Duncan et al (2020). In general, the approach is to sample observations according to an assumed 'true' model, and then use these in combination with the Log-Likelihood function to evaluate the ability to reproduce the assumed 'true' parameters. The simulation study consists of three steps:

(i) Postulate a true BBPS / BAPS model including specification and parameter values. For each relevant OD movement, identify a corresponding choice set of routes to be used for estimation.

(ii) Sample a set of observed route choices according to the true model using the specified link travel costs.

(iii) Apply MLE approach to obtain parameter estimates based on the observed route choices.

Step (ii) mimics estimating the models with tracked route observation data (e.g. GPS traces). The estimation procedure in principle needs to enumerate and store the universal choice sets in order to allow for evaluating the Log-likelihood for very large values of the bound $\varphi$ (e.g. in cases when the BBPS model approaches GPSL$'$ or the BAPS model approaches APSL). For larger networks this is not feasible and a subset consisting of routes with costs below some value being considerably larger than the bounding cost of the true model can be used.

The generic estimation procedure in Algorithm 1 is altered for simulation studies, by modifying **Step 1: Initialisation** as outlined in Algorithm 1 (Step 1) below to reflect (i) and (ii) in the above.

**Step 1: Initialisation.**

**1.1** Postulate a true set of parameters $(\boldsymbol{\alpha}^{true}, \theta_{true}, \beta_{true}, \varphi_{true}, \lambda_{true})$ for the BBPS model or $(\boldsymbol{\alpha}^{true}, \theta_{true}, \beta_{true}, \varphi_{true})$ for the BAPS model, and given these parameters generate/approximate the universal choice sets for OD movements $m = 1, \dots, M$, and store the link attributes and link-route information.

**1.2.**
BBPS model: Given the assumed true parameters and the generated choice sets, compute the BBPS model choice probabilities $\boldsymbol{P}_m$ for $m = 1, \dots, M$.
BAPS model: Given the assumed true parameters and the generated choice sets, solve each of the fixed-point problems

$$\boldsymbol{P}_m = \boldsymbol{F}_m\left(\boldsymbol{f}_m\left(\boldsymbol{c}_m\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha}^{true})\right)\right), \overline{\boldsymbol{\gamma}}_m^{BAPS}\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha}^{true}), \boldsymbol{P}_m\right); \theta_{true}, \beta_{true}, \varphi_{true}\right)$$

for $m = 1, \dots, M$.

**1.3.** Based on the BBPS model probabilities $\boldsymbol{P}_m$ or the BAPS model fixed-point choice probability solutions $\boldsymbol{P}_m^*$ for $m = 1, \dots, M$ (obtained in 1.2), sample $Z$ observed routes.

**1.4.** Define an initial set of parameter values $\left(\tilde{\boldsymbol{\alpha}}^{(1)}, \tilde{\theta}^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)}, \tilde{\lambda}^{(1)}\right)$ for the BBPS model or $\left(\tilde{\boldsymbol{\alpha}}^{(1)}, \tilde{\theta}^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)}\right)$ for the BAPS model for MLE, and set $n = 1$.

**Algorithm 1 (Step 1):** pseudo-code for initialisation of simulation experiments.

The number of observed routes to sample, $Z$, is exogenously defined. The robustness of the estimated parameters estimated can be investigated numerically by applying Algorithm 1 multiple times and then analysing the variation of the estimated parameters.

### 7.3.2 Sioux Falls Application

The Sioux Falls network consists of 76 links, 528 OD movements with non-zero travel demands, and 1,632,820 total routes. Details of the network were obtained from https://github.com/bstabler/TransportationNetworks. The travel cost of link $a$ is specified as the free-flow travel time $w_{a,1}$ only, such that:

$$t_a(\boldsymbol{w}_a;\boldsymbol{\alpha}) = w_{a,1} \cdot \alpha_1,$$

where $\alpha_1 > 0$ is the free-flow travel time parameter, and thus the travel cost for route $i \in R_m$ is:

$$c_{m,i}\left(\boldsymbol{t}(\boldsymbol{w};\boldsymbol{\alpha})\right) = \sum_{a \in A_{m,i}} t_a(\boldsymbol{w}_a;\boldsymbol{\alpha}) = \alpha_1 \sum_{a \in A_{m,i}} w_{a,1}.$$

The model requires the specification of four parameters: $\alpha_1$, $\theta$, $\beta$, and $\varphi$ but to ensure identification $\theta$ is fixed at $\theta = 1$ throughout.

Since the travel costs of the links (and thus routes) correspond to a single variable, to approximate the universal choice sets, we generate all routes with a free-flow travel time less than 2.5 times greater than the free-flow travel time on the quickest route for each OD movement (since the assumed true bound parameters are much less than 2.5). We also remove all OD movements where there are less than 5 routes. The result is that there are 370 remaining OD movements and a total of 42,976 routes, where the minimum, maximum, and average choice set sizes are 5, 898, and 116, respectively.

#### *7.3.2.1 BBPS Model Experiment Results*

We present results here from simulation studies estimating the BBPS$_{(\lambda=0)}$ model, and then investigate how estimating the $\lambda$ parameter effects simulation results.

The BBPS$_{(\lambda=0)}$ model Log-Likelihood function in (23) depends on three parameters $\alpha_1$, $\beta$, and $\varphi$, which can be visualised through three 3-dimensional projections of this 4-dimensional relationship. Fig. 8A-C display the BBPS$_{(\lambda=0)}$ model Log-Likelihood surface for a single estimation experiment, with $\alpha_1^{true} = 0.2$, $\beta_{true} = 1$, $\varphi_{true} = 1.5$ and $Z = 2000$. As Fig. 8A-C show, the Log-Likelihood surface is smooth and maximal around the true parameters, where the estimated parameters are $\hat{\alpha}_1 = 0.208 \pm 0.008$, $\hat{\beta} = 1.04 \pm 0.04$, and, $\hat{\varphi} = 1.5 \pm 0.002$.

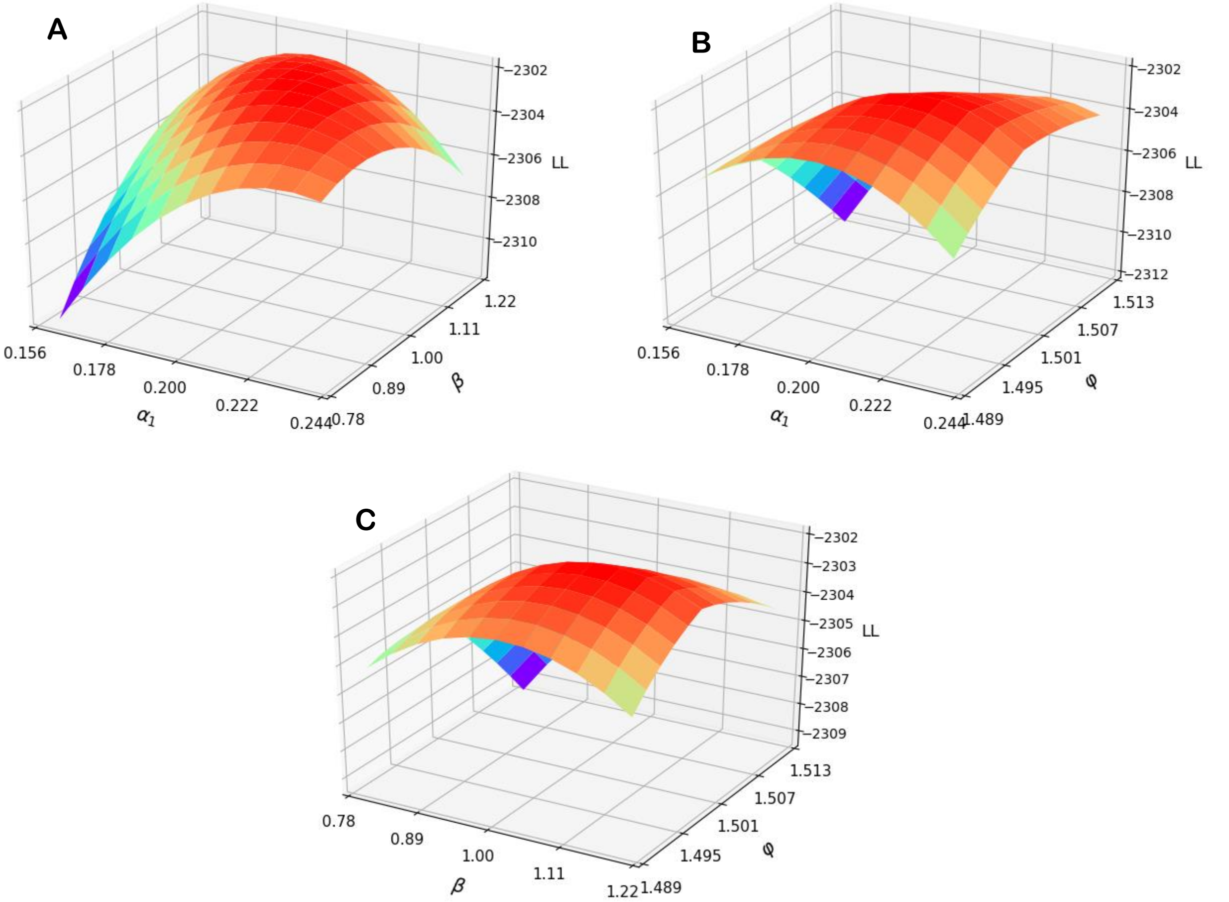



**Fig. 8.** Sioux Falls simulation study: BBPS$_{(\lambda=\theta)}$ Log-Likelihood surface ($\alpha_1^{true} = 0.2$, $\beta_{true} = 1$, $\varphi_{true} = 1.5$, $\hat{\alpha}_1 = 0.208$, $\hat{\beta} = 1.04$, $\hat{\varphi} = 1.5$). **A:** LL vs $(\alpha_1, \beta)$. **B:** LL vs $(\alpha_1, \varphi)$. **C:** LL vs $(\beta, \varphi)$.

Next, we investigate the stability of the estimated parameters for the BBPS$_{(\lambda=\theta)}$ model over multiple experiment replications. Each experiment utilises a Log-Likelihood maximisation algorithm (see Section 7.2.2) to obtain the parameter estimates with initial conditions $\left(\tilde{\alpha}_1^{(0)}, \tilde{\beta}^{(0)}, \tilde{\varphi}^{(0)}\right) = (0.15, 0, 1.1)$, and bounds $\tilde{\alpha}_1 \in [0,1]$, $\tilde{\beta} \in [0,2]$, $\tilde{\varphi} \in [1.01, 2.5]$.

Table 2 reports, for various settings of the true parameters, the mean Bias, Standard Error, and Route Mean Squared Error $\left(RMSE = \sqrt{(Bias)^2 + (S.E)^2}\right)$, of the estimates across $r = 25$ experiment replications with $Z = 1500$ simulated observations. Table 3 displays the estimated covariances between the $\alpha_1$, $\beta$, and $\varphi$ parameters. As shown, the mean bias of the estimates of $\alpha_1$, $\beta$, and $\varphi$ are small for all settings of the true parameters tested, with max absolute percentage biases of 7% ($\frac{0.014}{0.2} \times 100\%$), 6.4%, & 0.5%, respectively. There is thus no evidence of bias in the parameter estimates – the estimates are all close to the true values. However, as measured by the RMSE, the precision of estimating $\alpha_1$ and $\beta$ decrease as $\alpha_1^{true}$ and $\beta_{true}$ decrease. This seems reasonable as increasing $\alpha_1$ corresponds to lower perception error of travel cost and decreasing $\beta$ corresponds to lower perception of distinctiveness. Moreover, a lower perception error of travel cost also results in less precise estimations of the bound parameter $\varphi$ since fewer simulated observations are close to the bound. The RMSEs of the estimated bound parameters $\hat{\varphi}$ suggest though that the bound, at least for these settings of $\varphi_{true}$, can be estimated to a reasonably high level of precision.

Table 3 indicates that, with this network and the generated choice sets, there appears to be some negative correlation between the $\hat{\alpha}_1$ and $\hat{\beta}$ estimates since both scale negative utility components. There also appears to be some positive correlation between the $\hat{\alpha}_1$ and $\hat{\varphi}$ estimates, which is logical since both these parameters scale travel cost, where an increase in $\alpha_1$ or a decrease in $\varphi$ gives more probability to lower costing routes.

| $\alpha_1^{true}$ | $\beta_{true}$ | $\varphi_{true}$ | $\hat{\alpha}_1$ | | | $\hat{\beta}$ | | | $\hat{\varphi}$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Bias | S.E | RMSE | Bias | S.E | RMSE | Bias | S.E | RMSE |
| 0.2 | 0.8 | 1.5 | -0.008 | 0.031 | 0.0320 | -0.029 | 0.146 | 0.1489 | -0.003 | 0.0061 | 0.0068 |
| 0.2 | 1 | 1.4 | 0.002 | 0.027 | 0.0271 | -0.024 | 0.162 | 0.1638 | -0.004 | 0.0078 | 0.0088 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.2 | 1 | 1.5 | -0.014 | 0.023 | 0.0269 | 0.012 | 0.147 | 0.1475 | -0.008 | 0.0075 | 0.0110 |
| 0.2 | 1 | 1.6 | -0.001 | 0.017 | 0.0170 | 0.064 | 0.132 | 0.1467 | -0.001 | 0.0091 | 0.0092 |
| 0.1 | 1 | 1.5 | -0.007 | 0.028 | 0.0289 | -0.017 | 0.099 | 0.1004 | -0.004 | 0.0068 | 0.0079 |

**Table 2.** Sioux Falls simulation study: Stability of estimated BBPS$_{(\lambda=0)}$ parameters across multiple experiment replications ($Z = 1500$, $r = 25$).

| $\alpha_1^{true}$ | $\beta_{true}$ | $\varphi_{true}$ | $cov(\hat{\boldsymbol{\alpha}}_1, \hat{\boldsymbol{\beta}})$ | $cov(\hat{\boldsymbol{\alpha}}_1, \hat{\boldsymbol{\varphi}})$ | $cov(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\varphi}})$ |
|---|---|---|---|---|---|
| 0.2 | 0.8 | 1.5 | -0.00306 | 0.00007 | -0.00003 |
| 0.2 | 1 | 1.4 | -0.00045 | 0.00007 | 0.00082 |
| 0.2 | 1 | 1.5 | -0.00183 | 0.00004 | -0.00004 |
| 0.2 | 1 | 1.6 | -0.00085 | 0.00003 | 0.00042 |
| 0.1 | 1 | 1.5 | -0.00101 | 0.00010 | 0.00010 |

**Table 3.** Sioux Falls simulation study: Estimated covariances between BBPS$_{(\lambda=0)}$ model parameters from multiple experiments ($Z = 1500$, $r = 25$).

We also explore estimating the additional $\lambda$ parameter of the BBPS model. For the Log-Likelihood maximisation algorithm, the initial condition and bounds for $\lambda$ were $\tilde{\lambda}^{(0)} = 1$ and $\tilde{\lambda} \in [0,20]$, respectively. Table 4 displays for different settings of $\lambda_{true}$ the stability statistics of the estimates $\hat{\alpha}_1$, $\hat{\beta}$, $\hat{\varphi}$, and $\hat{\lambda}$ across $r = 25$ experiment replications with $Z = 1500$ simulated observations, where $\alpha_1^{true} = 0.2$, $\beta_{true} = 1$, and $\varphi_{true} = 1.5$. Table 4 also displays the estimated covariances between the $\alpha_1$ and $\lambda$ parameters. As shown, as measured by the MSE, the precision of estimating all parameters generally appears to decrease as $\lambda_{true}$ increases. Most notably, the precision of estimating $\lambda$ appears particularly poor for large $\lambda_{true}$, and the mean bias for $\lambda$ worsens as $\lambda_{true}$ increases where the percentage bias is 39% for $\lambda_{true} = 8$ and 34% for $\lambda_{true} = 10$, providing evidence of positive bias. There also appears to be some negative correlation between the $\hat{\alpha}_1$ and $\hat{\lambda}$ estimates, which makes sense since both scale travel cost within the path size contribution factors.

| $\lambda_{true}$ | $\hat{\alpha}_1$ | | | $\hat{\beta}$ | | | $\hat{\varphi}$ | | | $\hat{\lambda}$ | | | $cov(\hat{\boldsymbol{\alpha}}_1, \hat{\boldsymbol{\lambda}})$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Bias | S.E | RMSE | Bias | S.E | RMSE | Bias | S.E | RMSE | Bias | S.E | RMSE | |
| 2 | -0.014 | 0.032 | 0.0349 | -0.011 | 0.092 | 0.0927 | -0.007 | 0.008 | 0.0106 | 0.67 | 1.226 | 1.397 | -0.0347 |
| 5 | -0.014 | 0.042 | 0.0443 | 0.035 | 0.121 | 0.1260 | -0.006 | 0.010 | 0.0117 | 1.06 | 1.391 | 1.749 | -0.0397 |
| 8 | -0.028 | 0.044 | 0.0522 | 0.035 | 0.157 | 0.1609 | -0.009 | 0.008 | 0.0120 | 3.15 | 4.168 | 5.224 | -0.0647 |
| 10 | -0.024 | 0.043 | 0.0492 | 0.003 | 0.130 | 0.1300 | -0.008 | 0.011 | 0.0136 | 3.43 | 3.791 | 5.112 | -0.0899 |

**Table 4.** Sioux Falls simulation study: Stability of estimated BBPS model parameters across multiple experiment replications with different settings of $\lambda$ ($Z = 1500$, $r = 25$).

### 7.3.2.2 BAPS Model

#### 7.3.2.2.1 Experiment Results

The BAPS model Log-Likelihood function in (24) depends on three parameters $\alpha_1$, $\beta$, and $\varphi$, which can again be visualised through three 3-dimensional projections of this 4-dimensional relationship. Fig. 9A-C display the BAPS model Log-Likelihood surface for a single estimation experiment, with $\alpha_1^{true} = 0.2$, $\beta_{true} = 0.7$, $\varphi_{true} = 1.5$ and $Z = 2000$. As Fig. 9A-C show, the Log-Likelihood surfaces are smooth and approximately maximal around the true parameters, where the estimated parameters are $\hat{\alpha}_1 = 0.2 \pm 0.02$, $\hat{\beta} = 0.66 \pm 0.04$, and, $\hat{\varphi} = 1.496 \pm 0.004$.

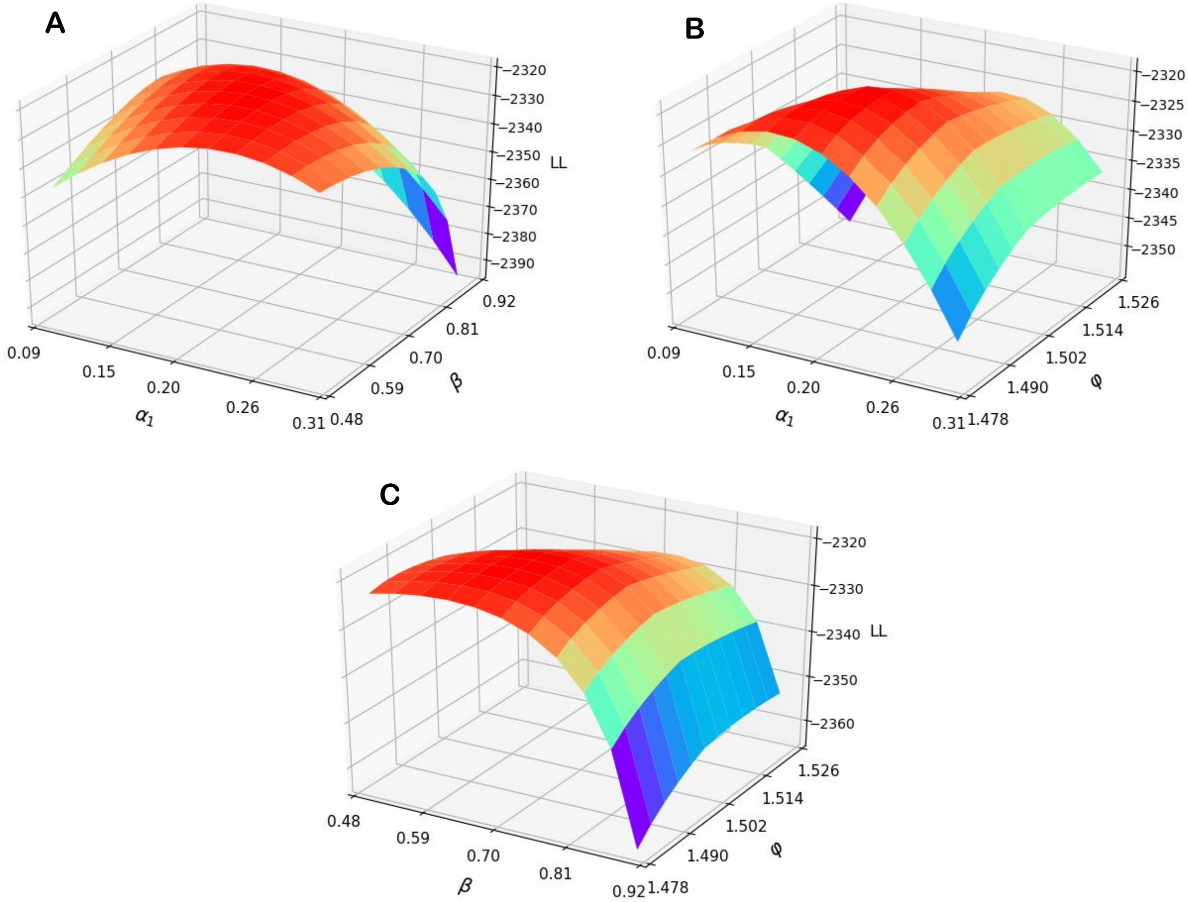



**Fig. 9.** Sioux Falls simulation study: BAPS model Log-Likelihood surface. ($\alpha_1^{true} = 0.2$, $\beta_{true} = 0.7$, $\varphi_{true} = 1.5$, $\hat{\alpha}_1 = 0.20$, $\hat{\beta} = 0.66$, $\hat{\varphi} = 1.496$). **A:** LL vs $(\alpha_1, \beta)$. **B:** LL vs $(\alpha_1, \varphi)$. **C:** LL vs $(\beta, \varphi)$.

Next, we investigate the stability of the estimated parameters over multiple experiment replications. Each experiment utilises a Log-Likelihood maximisation algorithm (see Section 7.2.2) to obtain the parameter estimates with initial conditions $\left(\tilde{\alpha}_1^{(0)}, \tilde{\beta}^{(0)}, \tilde{\varphi}^{(0)}\right) = (0.15,0,2)$, and bounds $\tilde{\alpha}_1 \in [0.05,1]$, $\tilde{\beta} \in [0,1]$, $\tilde{\varphi} = [1.01,2.5]$.

Table 5 reports, for various settings of the true parameters the mean bias, standard error, and RMSE of the estimates across $r = 25$ experiment replications with $Z = 1500$ simulated observations. Table 6 displays the estimated covariance between the $\alpha_1$, $\beta$, and $\varphi$ parameters. As shown, as for the BBPS model, the mean bias of the estimates of $\alpha_1$, $\beta$, and $\varphi$ are small for all settings of the true parameters tested, with max absolute percentage biases of 13%, 4.6%, & 0.6%, respectively. There is thus again no evidence of bias in the parameter estimates – the estimates are all close to the true values. The precision of estimating $\alpha_1$ and $\beta$ decrease as $\alpha_1^{true}$ and $\beta_{true}$ decrease, as anticipated. And, a lower perception error of travel cost again results in less precise estimations of the bound parameter $\varphi$. The RMSEs of $\hat{\beta}$ compared to those for the BBPS$_{(\lambda=\theta)}$ model in Table 2 suggest that the $\beta$ parameter can be estimated more accurately with the BAPS model. Table 6 indicates that there also appears to be some negative correlation between the $\hat{\alpha}_1$ and $\hat{\beta}$ estimates, as well as some positive correlation between the $\hat{\alpha}_1$ and $\hat{\varphi}$ estimates.

| $\alpha_1^{true}$ | $\beta_{true}$ | $\varphi_{true}$ | $\hat{\alpha}_1$ | | | $\hat{\beta}$ | | | $\hat{\varphi}$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Bias | S.E | RMSE | Bias | S.E | RMSE | Bias | S.E | RMSE |
| 0.2 | 0.8 | 1.5 | 0.000 | 0.018 | 0.0180 | 0.000 | 0.108 | 0.1080 | -0.003 | 0.0047 | 0.0056 |
| 0.2 | 0.7 | 1.4 | -0.004 | 0.030 | 0.0303 | -0.032 | 0.134 | 0.1378 | -0.004 | 0.0067 | 0.0078 |
| 0.2 | 0.7 | 1.5 | -0.003 | 0.014 | 0.0143 | -0.023 | 0.112 | 0.1143 | -0.004 | 0.0058 | 0.0070 |
| 0.2 | 0.8 | 1.7 | -0.004 | 0.017 | 0.0175 | 0.006 | 0.115 | 0.1152 | -0.002 | 0.0101 | 0.0103 |
| 0.1 | 0.7 | 1.5 | -0.013 | 0.022 | 0.0256 | 0.006 | 0.126 | 0.1261 | -0.004 | 0.0052 | 0.0066 |

**Table 5.** Sioux Falls simulation study: Stability of estimated BAPS model parameters across multiple experiment replications ($Z = 1500$, $r = 25$).

| $\alpha_1^{true}$ | $\beta_{true}$ | $\varphi_{true}$ | $cov(\widehat{\boldsymbol{\alpha}}_1, \widehat{\boldsymbol{\beta}})$ | $cov(\widehat{\boldsymbol{\alpha}}_1, \widehat{\boldsymbol{\varphi}})$ | $cov(\widehat{\boldsymbol{\beta}}, \widehat{\boldsymbol{\varphi}})$ |
|---|---|---|---|---|---|
| 0.2 | 0.8 | 1.5 | -0.00090 | 0.00004 | -0.00015 |
| 0.2 | 0.7 | 1.4 | -0.00198 | 0.00003 | 0.00029 |
| 0.2 | 0.7 | 1.5 | -0.00104 | 0.00002 | 0.00008 |
| 0.2 | 0.8 | 1.7 | -0.00104 | 0.00007 | 0.00026 |
| 0.1 | 1 | 1.5 | -0.00155 | 0.00005 | -0.00002 |

**Table 6.** Sioux Falls simulation study: Estimated covariance of BAPS model parameters from multiple experiment replications ($Z = 1500$, $r = 25$).

#### *7.3.2.2.2 Computation Analysis*

Due to the requirement of having to solve fixed-point problems to compute choice probabilities, in this subsection we analyse the computational performance of the BAPS model in the Sioux Falls MLE application. We The computer used has a 2.10GHz Intel Xeon CPU, 512GB RAM, and 64 Logical Processors (of which 50 were utilised). The code was implemented in Python. Results are reported throughout this section for a single simulation experiment where $Z = 1000$ route choice observations were simulated from the true model $\alpha_1^{true} = 0.2$, $\beta_{true} = 0.7$, $\varphi_{true} = 1.5$. $\hat{\alpha}_1 = 0.208$, $\hat{\beta} = 0.703$, and $\hat{\varphi} = 1.493$ were the consequent maximum likelihood estimates. Unless stated otherwise, the BAPS model choice probability convergence parameter $\xi$ was set as $\xi = 10$ (see Section 5.2.2).

Fig. 10A shows for different values of the BAPS model choice probability convergence parameter $\xi$ (and thus convergence statistic), the average number of fixed-point iterations per OD movement and computation time required to solve all of the 370 BAPS model fixed-point problems $\boldsymbol{P}_m = \boldsymbol{F}_m\left(\boldsymbol{f}_m\left(\boldsymbol{c}_m(\boldsymbol{t}), \overline{\boldsymbol{\gamma}}_m^{BAPS}(\boldsymbol{t}, \boldsymbol{P}_m)\right)\right)$, and consequently compute the Log-Likelihood value of the maximum likelihood estimates. As shown, computation time and average number of fixed-point iterations per OD increase roughly linearly as the convergence parameter is increased. As expected, computation times relate to the number of iterations required for convergence. Fig. 10B shows the value of the Log-Likelihood obtained as $\xi$ is increased. As shown, the Log-Likelihood increases in accuracy as the BAPS model choice probabilities become more accurate.

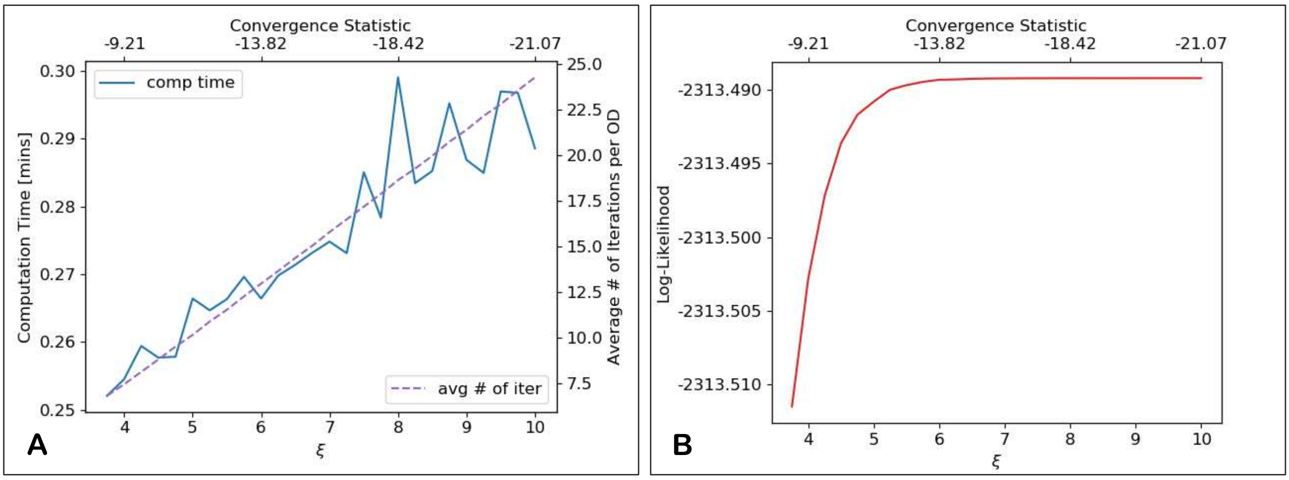



**Fig. 10.** Sioux Falls simulation study: Computational statistics for calculating a BAPS model Log-Likelihood as the BAPS model choice probability convergence parameter $\xi$ is increased. **A:** Average number of fixed-point iterations per OD / computation time [mins]. **B:** Log-Likelihood value.

Fig. 11 shows for different values of $\tilde{\varphi}$ the average number of fixed-point iterations per OD movement and computation time required to calculate the Log-Likelihood. As shown, the average number of iterations per OD required for convergence increases as $\tilde{\varphi}$ increases, and thus so do the required computation times. This is because the number of routes with a cost below the bound increases as the bound becomes less restrictive, and there are thus more routes to calculate the correlation between. This shows that the BAPS model can improve upon the computational performance of the APSL model in computing choice probabilities.

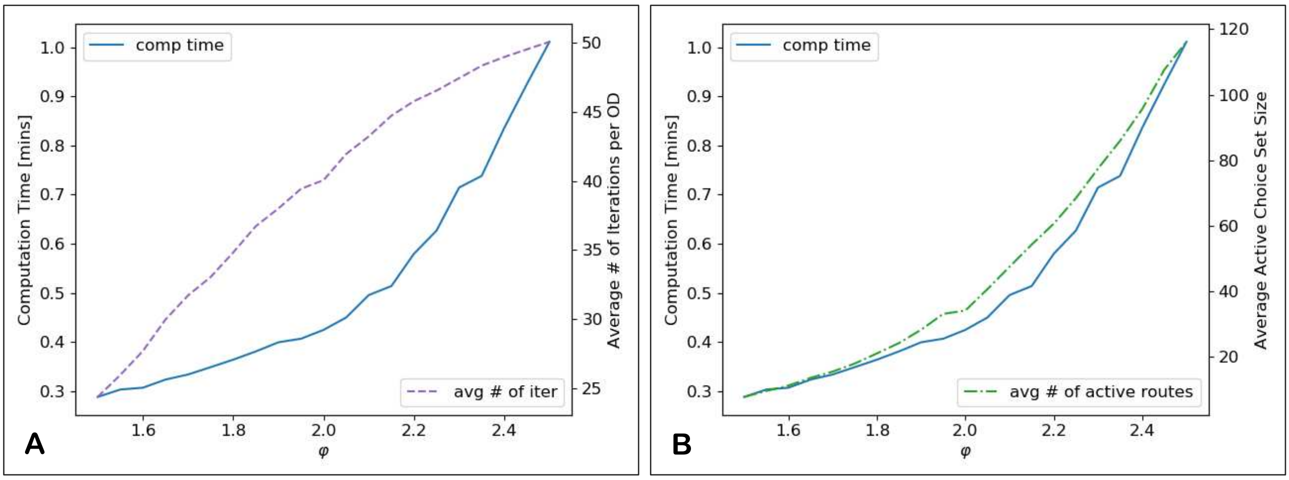



**Fig. 11.** Sioux Falls simulation study: Average number of fixed-point iterations (**A**) / active routes (**B**) per OD movement and computation time required to calculate the BAPS model Log-Likelihood for different $\tilde{\varphi}$ values.

Fig. 12A-B show for a single MLE (implementation of the L-BFGS-B algorithm), the cumulative computation times of the iterations and the BAPS model Log-Likelihood values and parameter estimates at the end of each iteration.

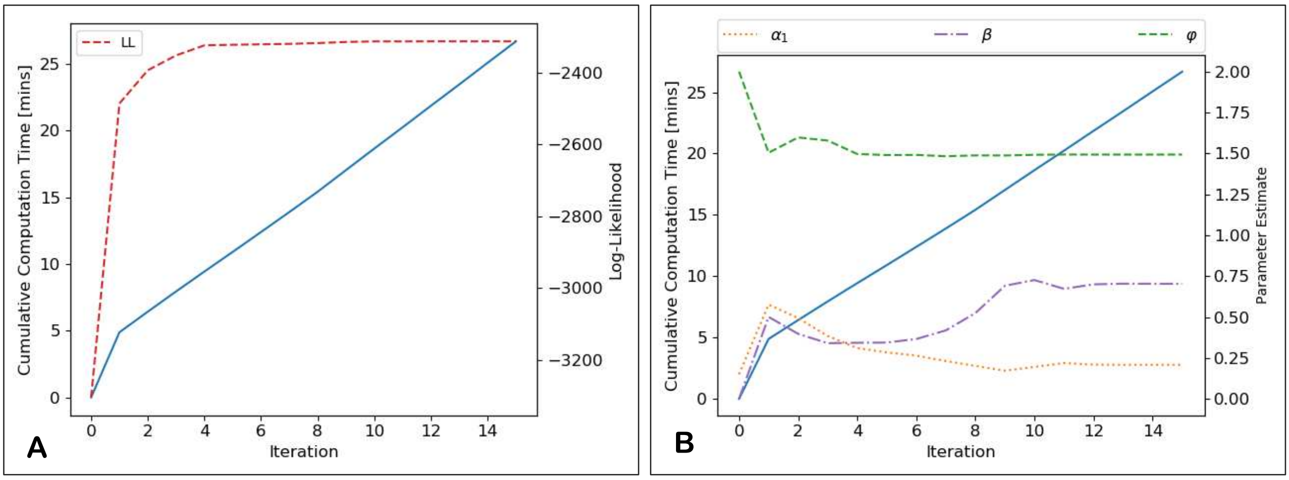



**Fig. 12.** Sioux Falls simulation study: Cumulative computation time at each iteration of a single BAPS model MLE, and MLE statistics. **A:** Log-Likelihood. **B:** Parameter estimates.

We also briefly investigate the impact of the $\tau$ parameter upon parameter estimation. For $\varphi = 1.5$, the largest choice set size is 898; thus, supposing that $\tau_m = \tau$, $m = 1, \ldots, M$, the maximum value for $\tau$ is $\frac{1}{898} \cong 10^{-3}$. Supposing $\tau$ assumes the form $\tau = 10^{-\nu}$, Fig. 13 displays how the maximum likelihood parameter estimates vary as $\nu$ varies. Unlike the APSL model, the BAPS model probability function is not continuous, and continuity is approximated by setting a small $\tau$ value. MLE requires a continuous probability function, and hence a small $\tau$ value is not only desired to approximate the standard formulation (like APSL), but is required so that the model is well behaved. For $\nu = 4$ and $\nu = 5$, MLE could not run successfully due to the discontinuity; however, as Fig. 13 shows for $\nu > 5$, MLE runs successfully and the parameter estimates are extremely close / roughly converge to the limit case of $\tau \to 0$. This demonstrates that we can recover the desired $\text{BAPS}_0$ model (Section 5.1) to a high computational accuracy using the BAPS model as defined in Section 5.2, with a sufficiently small value of $\tau$.

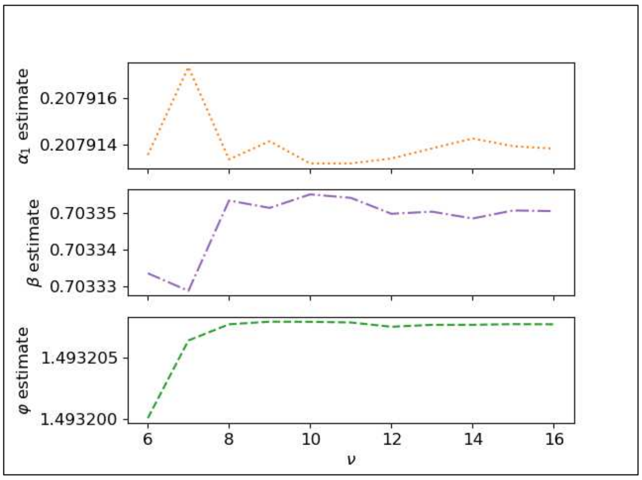
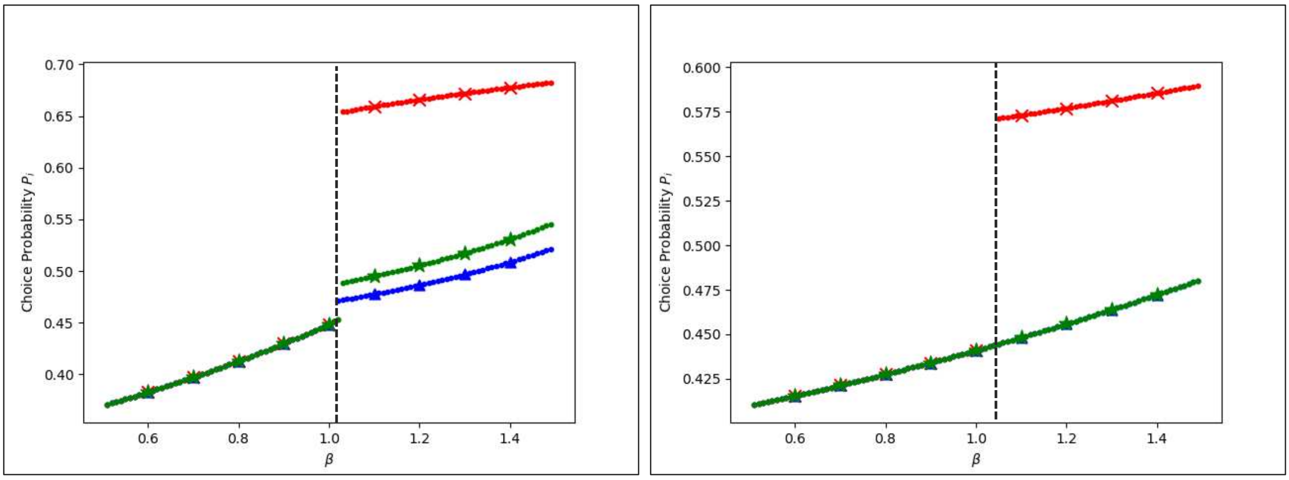



**Fig. 13.** Sioux Falls simulation study: Maximum likelihood BAPS model parameter estimates for different values of $\tau = 10^{-\nu}$.

### *7.3.2.2.3 BAPS Model Solution Uniqueness Analysis*

In this subsection we briefly investigate the uniqueness of BAPS model choice probability solutions in the context of the Sioux Falls simulation study. To do this, we utilise the method proposed in Section 10.3.4, where we plot trajectories of BAPS model solutions to approximate the uniqueness conditions, i.e. estimate $\beta_{max}$. A single simulation study is conducted for $\alpha_1^{true} = 0.2$, $\beta_{true} = 0.7$, $\varphi_{true} = 1.5$, and $Z = 2000$, leading to maximum likelihood estimates $\hat{\alpha}_1 = 0.200$, $\hat{\beta} = 0.747$, and $\hat{\varphi} = 1.499$ . We thus investigate whether BAPS model solutions are unique for these parameter estimates. Fig. 14 displays the maximum choice probability from three trajectories of BAPS model solutions as the $\beta$ parameter is varied for four different randomly chosen OD movements, with $\alpha_1 = \hat{\alpha}_1 = 0.200$ and $\varphi = \hat{\varphi} = 1.499$. $\beta$ was decremented by 0.01, and the initial large $\beta$ value was $\beta = 2$. As shown, the $\beta_{max,m}$ values ($\beta_{max}$ for OD movement $m$) for these OD movements can be estimated to vary between 0.86 and 0.94, suggesting that $\beta = 0.747$ results in universally unique solutions.



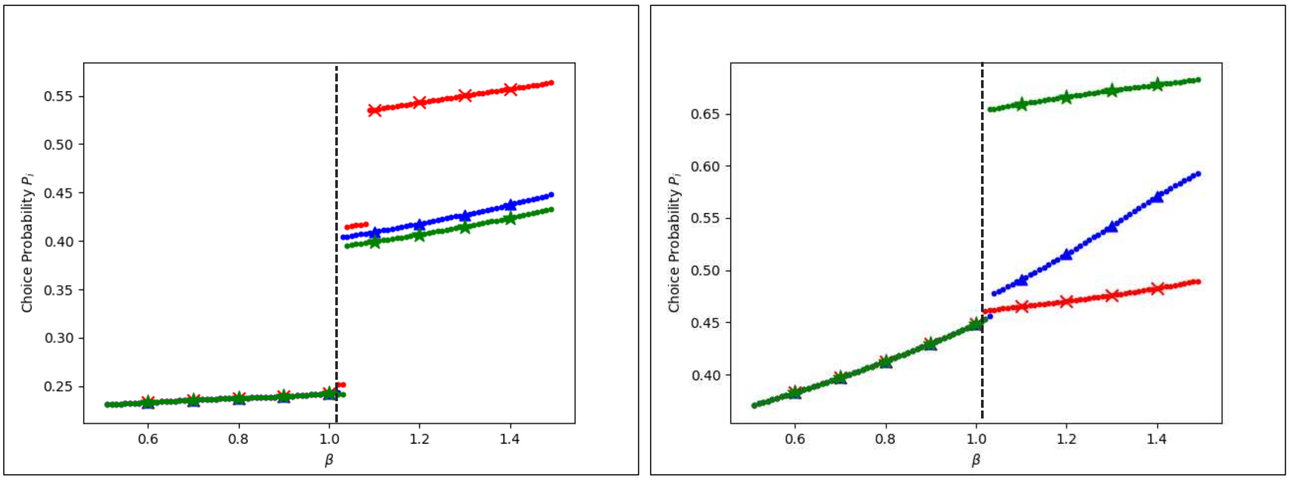



**Fig. 14.** Sioux Falls simulation study: Maximum choice probability of trajectories of BAPS model solutions as $\beta$ is varied.

#### *7.3.2.3 Model Robustness to the Adopted Choice Sets*

We briefly evaluate here on the Sioux Falls network the robustness of the BBPS & BAPS models to the adopted choice sets. Fig. 15A-B display the impact that varying the sizes of choice sets has on the route choice probabilities from the different models. The choice sets are generated using $k$-shortest path, with increasing values of $k$. It is assumed that the true active choice sets are those containing all routes with a free-flow travel time less than 2 and 2.5 times greater, respectively, than the free-flow travel time on the quickest route for each OD movement, and probability results are compared between these routes only (probability is zero if not generated). The model parameters are assumed known: $\alpha_1 = 0.2$, $\beta = 0.8$, $\lambda^{GPSL} = 10$, $\lambda^{BBPS} = 1$, and $\varphi = 2{,}2.5$ for Fig. 15A,B, respectively, and to compare the probability result $\boldsymbol{P}^{\{k\}}$ for the $k$-shortest path choice sets with the assumed true probabilities $\boldsymbol{P}^{true}$, we measure the Route Mean Squared Error (RMSE):

$$RMSE = \sqrt{\sum_{m=1}^{M} \sum_{i \in R_m} \left(P_{m,i}^{\{k\}} - P_{m,i}^{true}\right)^2 / N},$$

where $N$ is the total number of routes (12,844 for $\varphi = 2$, 42,976 for $\varphi = 2.5$). Fig. 16A-B show how the percentage of routes generated with a cost greater than the 2 and 2.5 relative cost bound varies, respectively, as $k$ varies, as well as the percentage of routes that should be generated but were not (non-generated routes with a relative cost less the bound).

As shown, the choice probability results for the MNL and PSL models both decrease in similarity to the respective assumed true probabilities as the choice sets are expanded and more unrealistic routes (with relative cost deviations greater than the bound) are present with the choice sets (shown in Fig. 16). The GPSL and APSL model results remain fairly stable in similarity due to the weighted contributions. The probability results for the bounded models, however, all increase in similarity since these models implicitly restrict the choice sets and perform better as more realistic routes are generated, regardless of how many generated unrealistic routes. As anticipated, GPSL & APSL are more robust than PSL due to the employment of path size contribution weighting techniques, while the BBPS & BAPS models are significantly more robust due to path size contribution elimination.

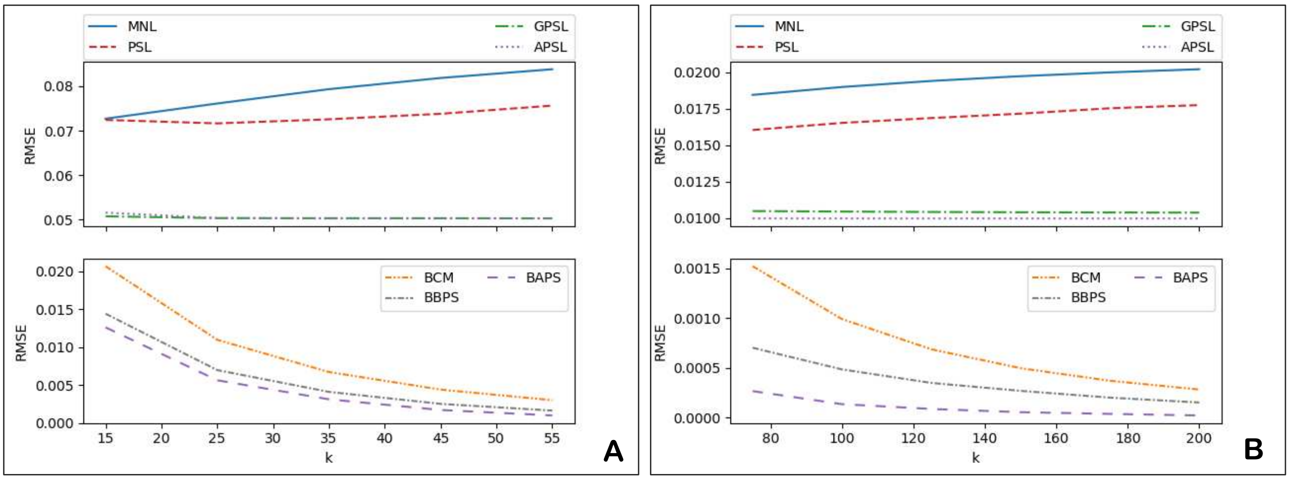


**Fig. 15.** Sioux Falls network: Impact that varying the sizes of choice sets has on the choice probabilities from different models, $k$-shortest path. **A:** $\varphi = 2$. **B:** $\varphi = 2.5$.

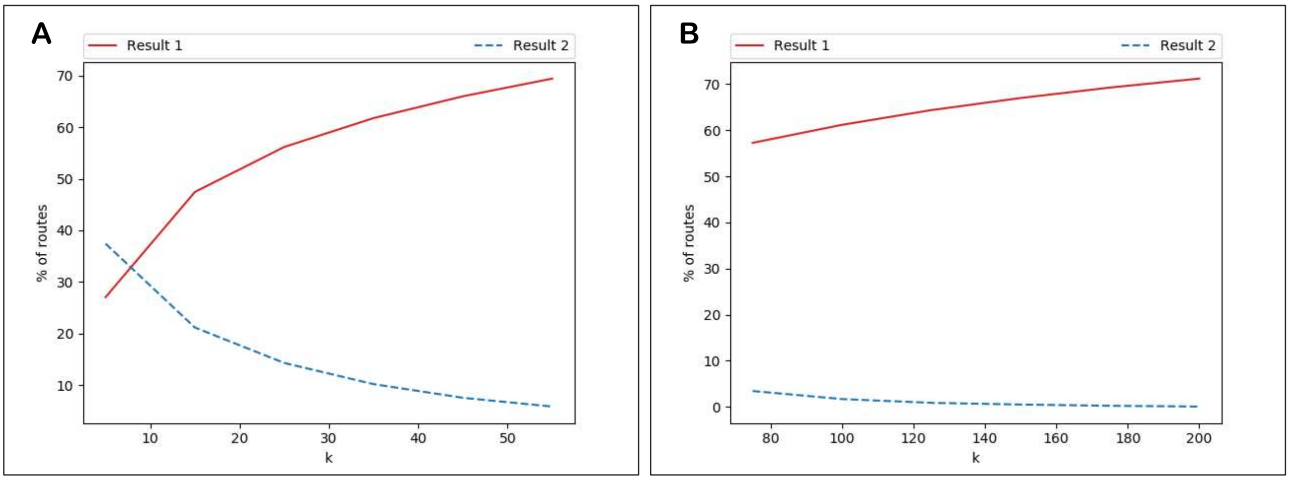



**Fig. 16.** Sioux Falls network: Percentage of routes in the choice sets with a free-flow travel time greater than or equal to the $\varphi$ relative cost bound (Result 1) and percentage of routes that should be generated but were not as $k$ varies (Result 2). **A:** $\varphi = 2$. **B:** $\varphi = 2.5$.

## 7.4 Real-Life Large-Scale Case Study

In this section we estimate the BBPS and BAPS models, where the model parameters are estimated using MLE with observed route choices tracked by GPS units. The data has been collected among drivers in the eastern part of Denmark in 2011, and includes a total of 17,115 observed routes. The dataset is the same as used in Prato et al (2014), Rasmussen et al (2017), and Duncan et al (2020), and after a filtering to include only trips where the sum of travel time (in minutes) and length (in km) is at least 10, a total of 8,696 observations remain.

The GPS traces are map matched to a network, for which corresponding time-of-day dependent travel times are available on the entire network. See more details in Prato et al (2014). The network is large-scale, representing all of Denmark, and thus includes 34,251 links. With current alternative generation techniques, it is not feasible to enumerate the universal choice set for such a large network, and even enumerating all alternatives with a cost below a rather large relative bound (e.g. $\varphi = 2$) is not feasible. Instead, we approximate the universal choice set by generating a choice set for each observed route by applying the doubly stochastic approach also applied in Prato et al (2014). This approach is based on repeated shortest path search in which the network attributes and parameters of the cost function are perturbated between searches (Nielsen, 2000; Bovy & Fiorenzo-Catalano, 2007). To reduce the risk of bias in estimation, care was taken to ensure a large variety of alternatives with different characteristics were generated, by assuming large variance in the parameters of the cost function. Up to 100 unique paths are generated for each observation, and for 591 observations only the observed route was generated, so these are removed from the data set, leaving 8105 observations.

For the estimation, the travel cost of link $a$ is specified as a weighted sum of congested travel time $w_{a,1}$ (in minutes), and length $w_{a,2}$ (in kilometres), such that:

$$t_a(\boldsymbol{w}_a; \boldsymbol{\alpha}) = w_{a,1} \cdot \alpha_1 + w_{a,2} \cdot \alpha_2$$

where $\alpha_1 > 0$ and $\alpha_2 > 0$ are the congested travel time, and length parameters, respectively. The generalised travel cost for route $i \in R_m$ is thus:

$$c_{m,i}\big(\boldsymbol{t}(\boldsymbol{w}; \boldsymbol{\alpha})\big) = \sum_{a \in A_{m,i}} t_a(\boldsymbol{w}_a; \boldsymbol{\alpha}) = \sum_{a \in A_{m,i}} \big(w_{a,1} \cdot \alpha_1 + w_{a,2} \cdot \alpha_2\big) = \alpha_1 \sum_{a \in A_{m,i}} w_{a,1} + \alpha_2 \sum_{a \in A_{m,i}} w_{a,2}.$$

The model requires the specification of five parameters: $\alpha_1$, $\alpha_2$, $\theta$, $\beta$, and $\varphi$ but to ensure identification, the $\theta$ parameter is fixed at $\theta = 1$. There are some outlying observations in the data where the relative travel time / length deviation of the observed route away from the quickest/shortest route is high. So that the estimation results are not influenced significantly by these outliers, and to improve the analysis of results, we remove 82 route observations where either the relative travel time or length deviation is over 1.5, leaving 8023 observations, see the distribution of the choice set sizes in Fig. 17.

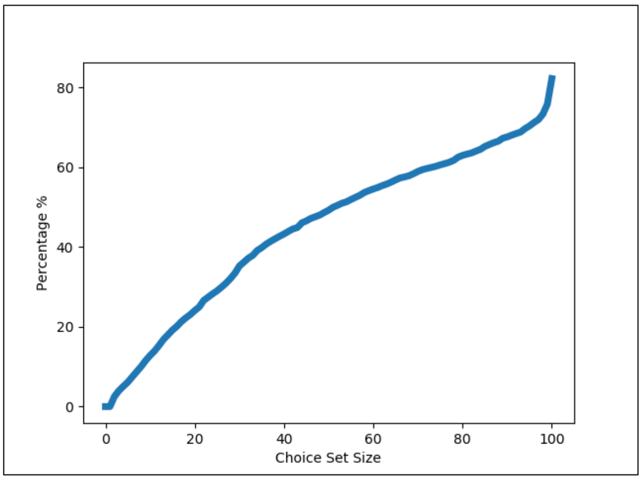



**Fig. 17.** Real-life case-study: Cumulative distribution of the choice set sizes for the 8,023 observations.

Fig. 18A shows the relative travel time deviations away from the quickest routes in the choice sets for the observed routes as well as the alternative routes generated, and Fig. 18B shows the relative length deviations.

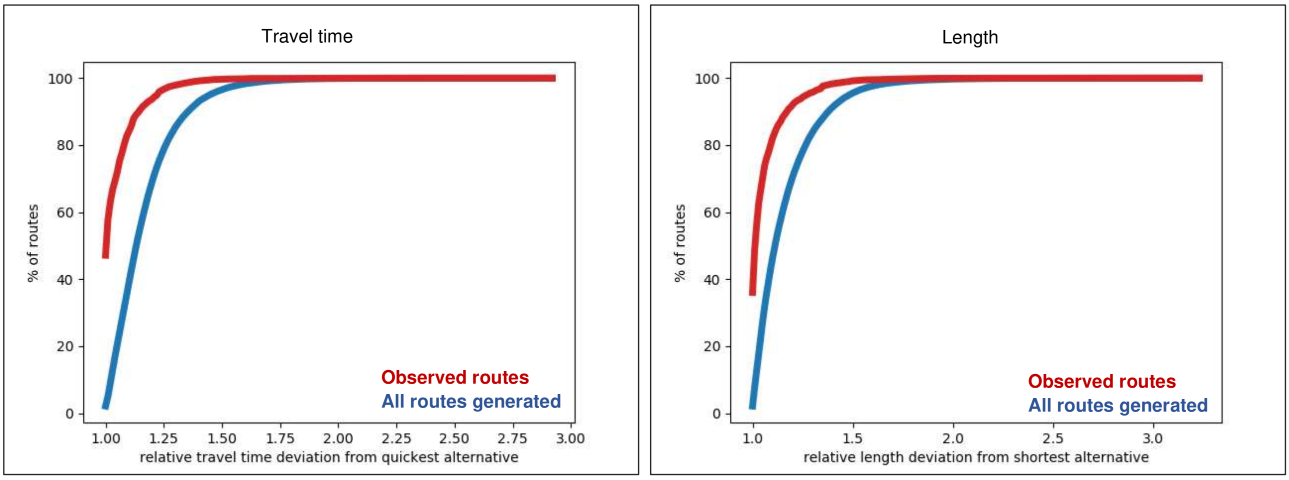



**Fig. 18.** Real-life case-study: Relative deviations away from quickest/shortest routes in the choice sets for the observed routes (red) and alternative routes generated (blue).

We estimate the models utilising the same Log-Likelihood maximisation algorithm (L-BFGS-B, see Section 7.2.2), initial conditions, and parameter bounds, where appropriate. Initial conditions are: $\left(\tilde{\alpha}_1^{(1)}, \tilde{\alpha}_2^{(1)}, \tilde{\beta}^{(1)}, \tilde{\varphi}^{(1)}, \tilde{\lambda}^{(1)}\right) = (0.5,0.5,0,1.6,0)$, and bounds: $\tilde{\alpha}_1, \tilde{\alpha}_2 \in [0,1]$, $\tilde{\beta} \in [0,2]$, $\tilde{\varphi} \in [1.01,5]$, $\tilde{\lambda} \in [0,200]$. For the APSL and BAPS models the bounds are: $\tilde{\alpha}_1, \tilde{\alpha}_2 \in [0.1,1]$, $\tilde{\beta} \in [0,1]$, $\tilde{\varphi} \in [1.01,5]$.

### 7.4.1 BBPS Model Estimation

Table 7 displays the BBPS$_{(\lambda=0)}$ and BBPS model parameter estimates, and the consequent Log-Likelihood values. The BBPS model appears to outperform the BBPS$_{(\lambda=0)}$ model due to the greater flexibility the $\lambda$ parameter provides; however, the estimated bound is very large considering the relative deviations in Fig. 18, which results in every route having a cost within the bound and the BBPS approximating the GPSL$'$ model. This suggests that the GPSL$'$ model with a large $\lambda$ value is outperforming more internally consistent models by capturing something other than the correlation between the realistic routes. We explore this further in Section 7.4.3.

| | $\hat{\alpha}_1$ | $\hat{\alpha}_2$ | $\hat{\beta}$ | $\hat{\lambda}$ | $\hat{\varphi}$ | $LL$ |
|---|---|---|---|---|---|---|
| BBPS$_{(\lambda=0)}$ | 0.690 | 0.209 | 1.786 | | 1.495 | -18556 |
| BBPS | 0.433 | 0.148 | 0.970 | 10.277 | 3.834 | -17463 |

**Table 7.** Real-life case-study: BBPS$_{(\lambda=0)}$ & BBPS parameter estimates and Log-Likelihood values.

Fig. 19A-F visualise the BBPS$_{(\lambda=\theta)}$ model Log-Likelihood surface around the four parameter estimates; as can be seen, these are smooth.

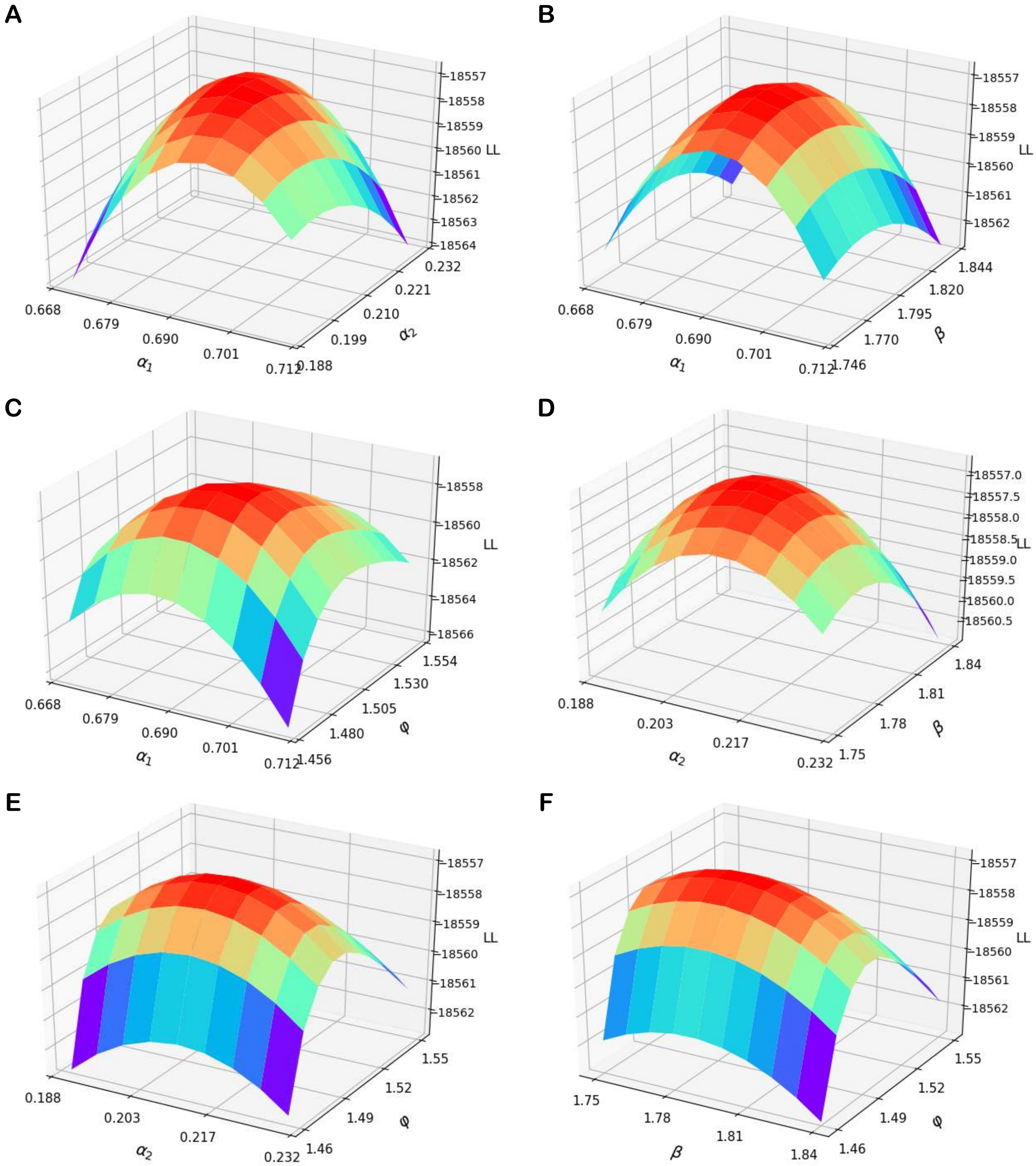



**Fig. 19.** Real-life case-study: BBPS$_{(\lambda=\theta)}$ model Log-Likelihood surface around parameter estimates in Table 7. **A:** LL vs $(\alpha_1, \alpha_2)$. **B:** LL vs $(\alpha_1, \beta)$. **C:** LL vs $(\alpha_1, \varphi)$. **D:** LL vs $(\alpha_2, \beta)$. **E:** LL vs $(\alpha_2, \varphi)$. **F:** LL vs $(\beta, \varphi)$.

### 7.4.2 BAPS Model Estimation

#### *7.4.2.1 Results*

Table 8 displays the BAPS model parameter estimates and the consequent Log-Likelihood value. As shown, the estimates all seem reasonable and the BAPS model appears to provide better fit over the BBPS$_{(\lambda=\theta)}$ model in Table 7.

| $\hat{\alpha}_1$ | $\hat{\alpha}_2$ | $\hat{\beta}$ | $\hat{\varphi}$ | $LL$ |
|---|---|---|---|---|
| 0.629 | 0.250 | 0.844 | 1.506 | -18308 |

**Table 8.** Real-life case-study: BAPS model parameter estimates and Log-Likelihood.

Fig. 20A-F visualise the Log-Likelihood surface around the four parameter estimates; as can be seen, these are smooth.

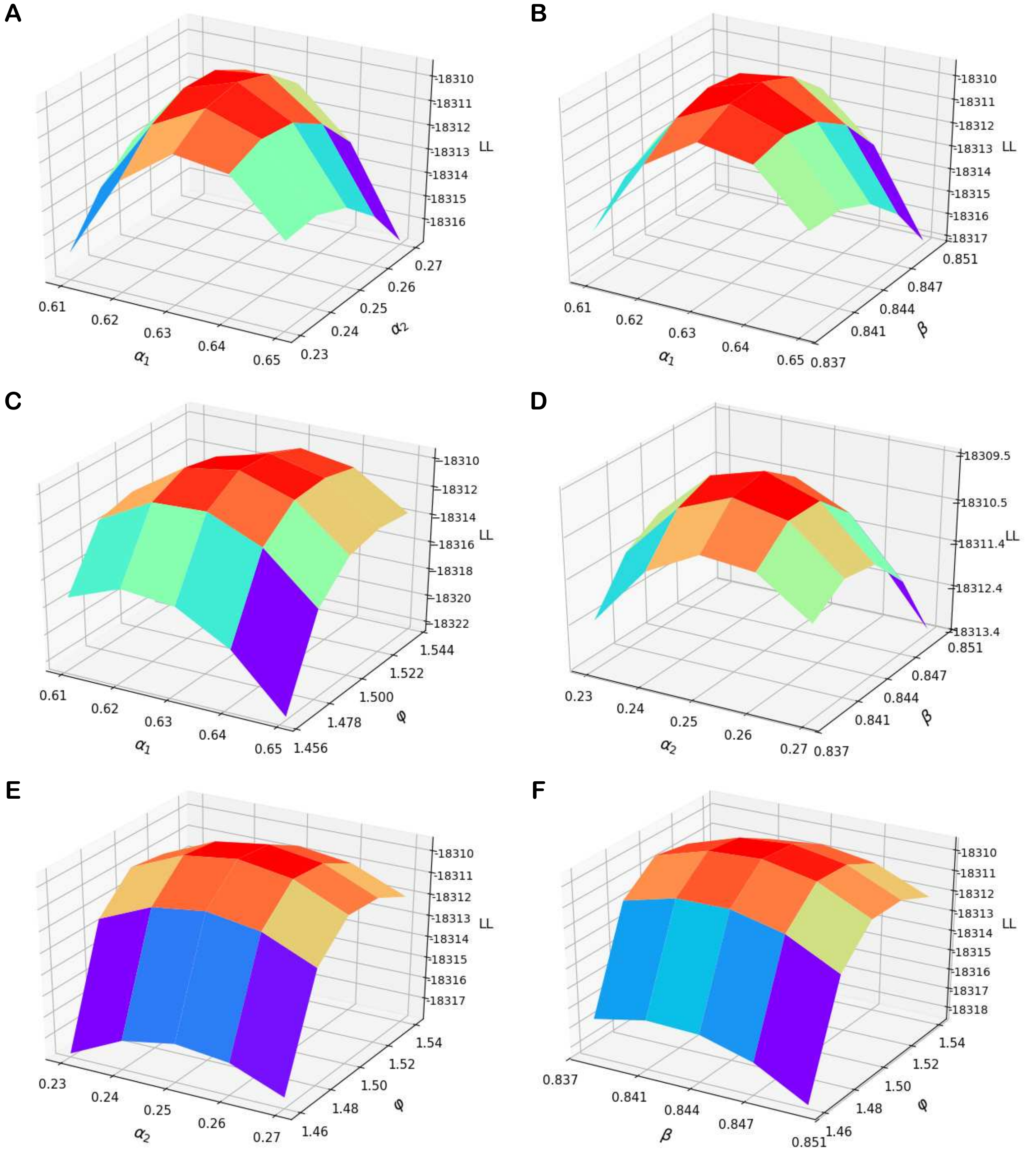



**Fig. 20.** Real-life case-study: BAPS model Log-Likelihood surface around parameter estimates in Table 8. **A:** LL vs $(\alpha_1, \alpha_2)$. **B:** LL vs $(\alpha_1, \beta)$. **C:** LL vs $(\alpha_1, \varphi)$. **D:** LL vs $(\alpha_2, \beta)$. **E:** LL vs $(\alpha_2, \varphi)$. **F:** LL vs $(\beta, \varphi)$.

#### *7.4.2.2 Computation Analysis*

We analyse here the computational performance of the BAPS model in the real-life case study. The same computer was used as in Section 7.3.2.2.2. Unless stated otherwise, the BAPS model choice probability convergence parameter $\xi$ was set as $\xi = 7$.

Fig. 21A shows for different values of the BAPS model choice probability convergence parameter $\xi$ (and thus convergence statistic), the average number of fixed-point iterations per OD movement and computation time required to solve all of the 8,023 BAPS model fixed-point problems $\boldsymbol{P}_{m_z} = \boldsymbol{F}_{m_z}\left(\boldsymbol{f}_{m_z}\left(\boldsymbol{c}_{m_z}(\boldsymbol{t}), \overline{\boldsymbol{\gamma}}^{BAPS}_{m_z}\left(\boldsymbol{t}, \boldsymbol{P}_{m_z}\right)\right)\right)$ for $z = 1, \ldots, Z$, and consequently compute a single Log-Likelihood, with the estimated BAPS model parameters in Table 8. Fig. 21B shows the value of the Log-Likelihood obtained as $\xi$ is increased. As shown, computation time and average number of fixed-point iterations per OD increase linearly as the convergence parameter is increased, and the Log-Likelihood increases in accuracy (from $\xi = 2$) as the BAPS model choice probabilities become more accurate.

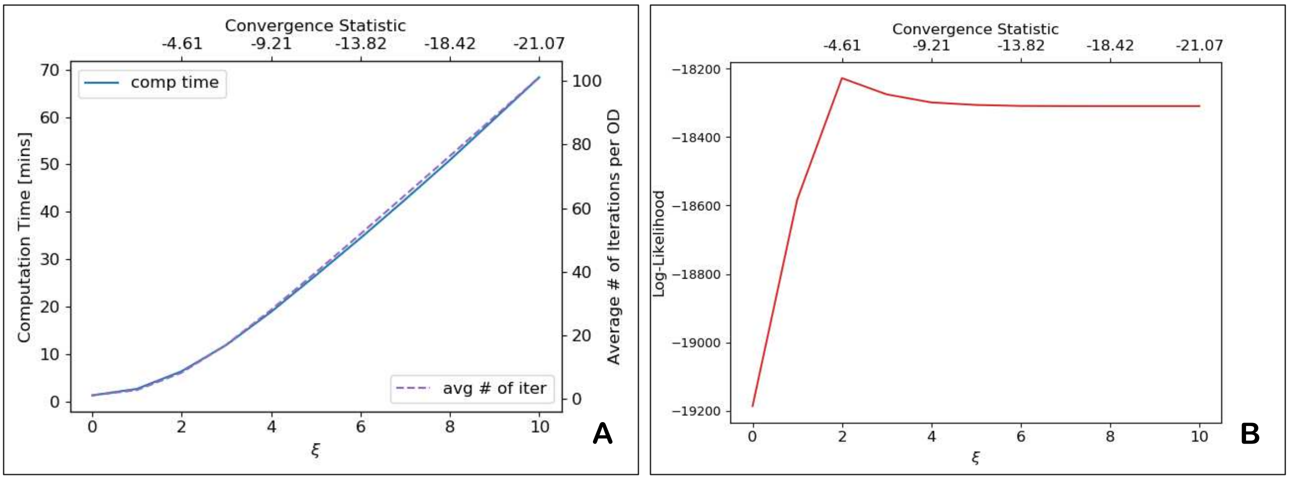



**Fig. 21.** Real-life case-study: Computational statistics for calculating the estimated BAPS model Log-Likelihood as the BAPS model choice probability convergence parameter $\xi$ is increased. **A:** Average number of fixed-point iterations per OD / computation time [mins]. **B:** Log-Likelihood value.

Fig. 22A shows for different values of $\varphi$ the average number of fixed-point iterations per OD movement and computation time required to solve the BAPS model, with $\alpha_1$, $\alpha_2$, and $\beta$ set as the estimated BAPS model parameters in Table 8. Fig. 22B shows the average active choice set size as $\varphi$ increases. As shown, the average number of iterations per OD required for convergence and average active choice set size increases as $\varphi$ increases, and thus so do the required computation times.

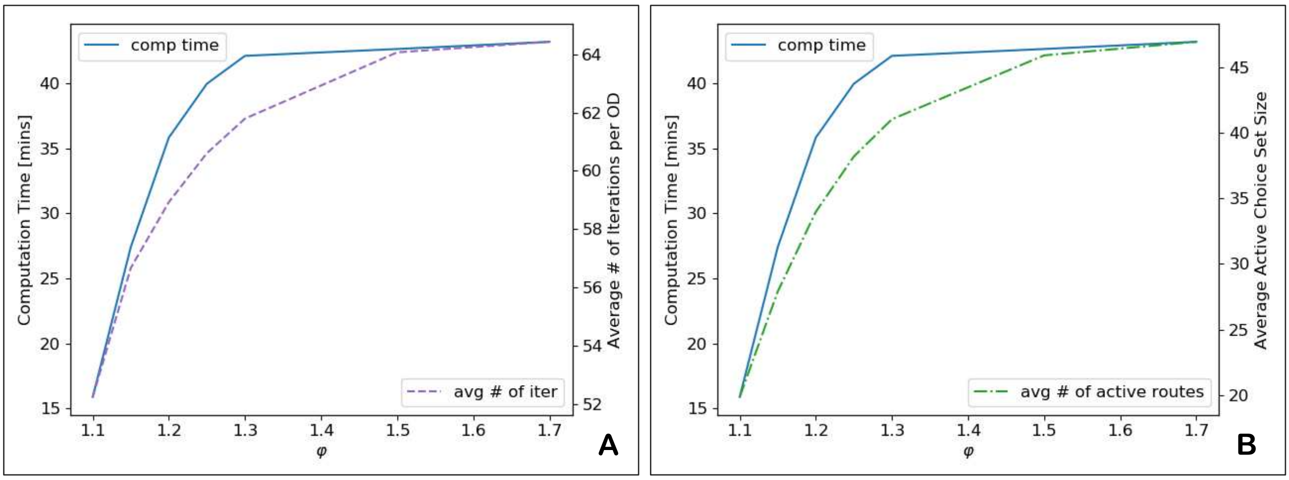



**Fig. 22.** Real-life case study: The impact of $\varphi$ on computation statistics for solving the BAPS model with $\alpha_1$, $\alpha_2$, $\beta$ as the parameter estimates in Table 8. Computation time [mins] and **A:** Average number of fixed-point iterations per OD movement. **B:** Average active choice set size.

Fig. 23A-B show for a single estimation of the BAPS model (implementation of the L-BFGS-B algorithm), the cumulative computation times of the iterations and the Log-Likelihood values and parameter estimates at the end of each iteration, respectively.

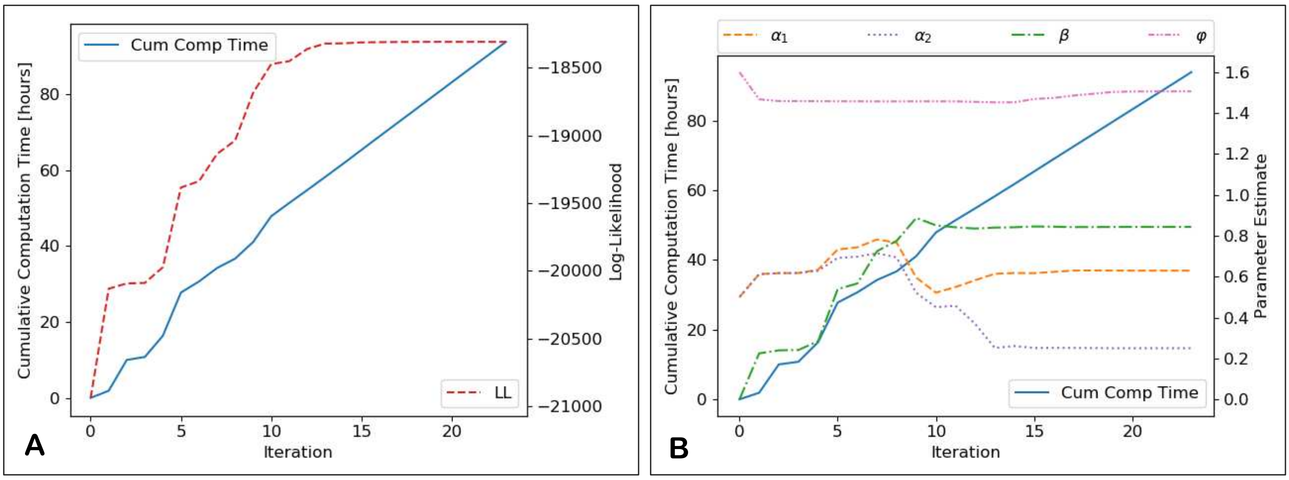



**Fig. 23.** Real-life case-study: Cumulative computation time at each iteration for a single estimation of the BAPS model, and MLE statistics. **A:** Log-Likelihood. **B:** Parameter estimates.

### *7.4.2.3 BAPS Model Solution Uniqueness Analysis*

We briefly investigate here the uniqueness of BAPS model choice probability solutions in the context of the real-life case study. Similar to the experiments conducted in Section 7.3.2.2.3 for the Sioux Falls simulation study, we estimate the uniqueness conditions for the network given the estimated parameters. Trajectories of BAPS model solutions are plotted to approximate $\beta_{max}$. Fig. 24 displays the maximum choice probability from trajectories of BAPS model solutions as the $\beta$ parameter is varied for four different randomly chosen OD movements, with $\alpha_1$, $\alpha_2$, and $\varphi$ as in Table 8. $\beta$ was decremented by 0.01, and the initial large $\beta$ value was $\beta = 1.5$. As shown, the $\beta_{max,m}$ values for these OD movements are around 1, suggesting that $\beta = 0.844$ results in universally unique solutions.

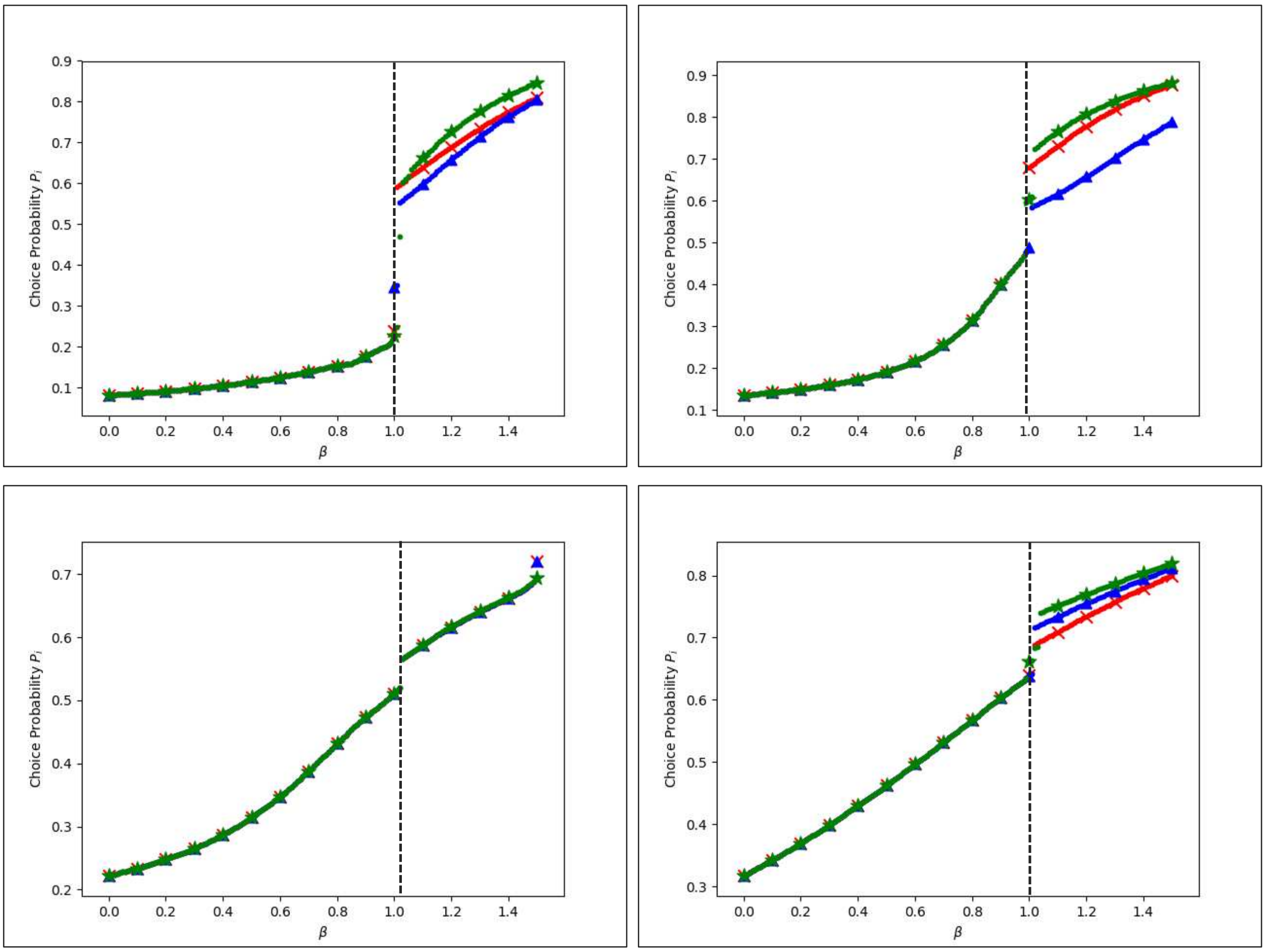



**Fig. 24.** Real-life case study: Maximum choice probability from trajectories of BAPS model solutions as $\beta$ is varied.

### 7.4.3 Comparing Results with Other Models

In this subsection we estimate models discussed in this paper and compare results. Table 9 shows the estimated parameters and Log-Likelihood values for the MNL, PSL, GPSL, GPSL′, GPSL′$_{(\lambda=\theta)}$, & APSL models, as well as the BCM, BBPS$_{(\lambda=\theta)}$, BBPS, & BAPS models. As anticipated, the estimated bounds for the BCM, and BBPS$_{(\lambda=\theta)}$ and BAPS models are all around 1.5; however, the estimated bound for the BBPS model is much larger than 1.5 and while the given value is 3.834 it is approximating $\varphi \to \infty$ where the BBPS model collapses to the GPSL′ model, which is evident from the same estimated parameters and Log-Likelihood value. We discuss this result in more detail below.

| | $\hat{\alpha}_1$ | $\hat{\alpha}_2$ | $\hat{\beta}$ | $\hat{\lambda}$ | $\hat{\varphi}$ | $LL$ |
|---|---|---|---|---|---|---|
| MNL | 0.799 | 0.441 | | | | -20573 |
| PSL | 0.990 | 0.405 | 1.335 | | | -19907 |
| GPSL | 0.431 | 0.126 | 1.133 | 103.89 | | -17327 |
| GPSL′ | 0.433 | 0.148 | 0.970 | 10.277 | | -17463 |
| GPSL′$_{(\lambda=\theta)}$ | 0.701 | 0.212 | 1.780 | | | -18571 |
| APSL | 0.642 | 0.251 | 0.842 | | | -18323 |
| BCM | 0.786 | 0.439 | | | 1.486 | -20565 |
| BBPS$_{(\lambda=\theta)}$ | 0.690 | 0.209 | 1.786 | | 1.495 | -18556 |
| BBPS | 0.433 | 0.148 | 0.970 | 10.277 | 3.834 | -17463 |
| BAPS | 0.629 | 0.250 | 0.844 | | 1.506 | -18308 |

**Table 9.** Real-life case-study: Estimation results.

To compare the fits of the estimated models, Table 10 shows the penalised-likelihood criteria. As expected, the MNL model provides the worst fit, and the Path Size models all perform significantly better. APSL outperforms GPSL′$_{(\lambda=\theta)}$ and the BAPS model outperforms the BBPS$_{(\lambda=\theta)}$ model suggesting that internal consistency can improve model fit, but more specifically by including a measure of distinctiveness within the path size contribution factors. By applying a relative bound of around 1.5 to the route costs, the BCM, and BBPS$_{(\lambda=\theta)}$ & BAPS models all improve upon the fit of their limit models MNL, GPSL′$_{(\lambda=\theta)}$, and APSL, respectively, showing the value in excluding the influence of unrealistic routes. The BBPS model, however, cannot improve upon the fit of its limit model despite it being known that unrealistic routes are present in the choice sets.

GPSL and GPSL′ (also BBPS with $\varphi \to \infty$) outperform all models, however this appears not to be by design. The PSL′ model introduced by Ben-Akiva & Bierlaire (1999) and then the GPSL model by Ramming (2002) were constructed so that, as Ramming (2002) notes, "arbitrarily long paths – which would likely not be considered by travelers – do not reduce the size of other, more reasonable paths that use the same link", which loosely translates as so that the path size terms are attempting the capture the correlation between the realistic alternatives only. So, if these models are aiming to reduce the contributions of unrealistic routes to the path size terms of realistic routes, then eliminating the contributions completely should improve performance. However, when the GPSL′ model is given the opportunity to eliminate contributions, i.e. with the BBPS model, the option is not taken, and the best fit comes from an unbounding $\varphi$ and a large $\lambda$ value. This clearly indicates that the GPSL and GPSL′ models are able to provide better fits to real data by capturing something other than the correlation between the realistic routes within the path size terms.

Duncan et al (2020) estimate the GPSL model with the same data set but without excluding the 82 route observations with relatively large travel times / lengths. As they note, the data set contains relatively costly but relatively universally distinct route observations (i.e. without considering whether or not the routes are link sharing with unrealistic alternatives), and the GPSL model is able to provide the best fit for these observations, without compromising the fit for the low costing observations. The GPSL travel cost parameter estimates are smaller than the same estimates for the other models, which improves the relative attractiveness of the costly alternatives. To counterbalance this so that that the low costing routes still remain attractive, GPSL introduces a large $\lambda$ value: routes with relatively small travel costs are penalised significantly less than routes with relatively large travel costs for link sharing. Moreover, GPSL is able to further increase the relative attractiveness of the distinct, costly routes by decreasing the attractiveness of the indistinct, costly routes with the large $\lambda$. It appears then that for the GPSL and GPSL′ models to work well, they require the presence of costly routes in the choice sets so that the counterbalancing can occur, which is why the bound is all-inclusive.

What is noticeable about the estimated GPSL parameters with this reduced data set is that the travel cost parameters are slightly larger (than $\hat{\alpha}_1 = 0.415$ and $\hat{\alpha}_1 = 0.085$ from full data set), which make sense since the most relatively costly observations have been removed. The estimated $\lambda$ parameter is also larger (than $\hat{\lambda} = 91.95$) which fits with the arguments above: a larger $\lambda$ is required to counterbalance the small travel cost parameters (but greater than before) for the low costing routes.

Furthermore, as reported in Section 7.3.2.1 in the Sioux Falls simulation experiments, larger values of $\lambda$ for the BBPS model makes estimation more unreliable/unstable. Due to the clear similarities with analogous additional $\lambda$ parameters, it would be natural to assume that this is also the case for the GPSL models, further adding to the undesirability of estimating GPSL/BBPS with large $\lambda$.

The reason why the relative improvement in fit from BCM to BBPS$_{(\lambda=\theta)}$ is greater than from MNL to PSL is because PSL does not deal with unrealistic routes in the path size terms at all. It is therefore not just limited in how it can adjust for correlation compared to the bounded path size models, but also the weighted path size contribution models. When comparing relative improvement in fit from the BCM to BBPS$_{(\lambda=\theta)}$ with MNL to GPSL$'_{(\lambda=\theta)}$ (the limit model of BBPS$_{(\lambda=\theta)}$), however, the effects are of the same order of magnitude, across the range of tests i.e. for the primary estimation results in Table 9&Table 10 and re-estimation results below in Table 11.

| | AIC | BIC | CAIC |
|---|---|---|---|
| MNL | 41150 | 41164 | 41166 |
| PSL | 39820 | 39841 | 39844 |
| GPSL | 34662 | 34690 | 34694 |
| GPSL$'$ | 34934 | 34961 | 34966 |
| GPSL$'_{(\lambda=\theta)}$ | 37148 | 37168 | 37172 |
| APSL | 36652 | 36673 | 36676 |
| BCM | 41136 | 41157 | 41160 |
| BBPS$_{(\lambda=\theta)}$ | 37120 | 37148 | 37152 |
| BBPS | 34936 | 34970 | 34976 |
| BAPS | 36624 | 36651 | 36656 |

**Table 10.** Real-life case-study: Comparison of fit between models based on penalised-likelihood criteria.

As shown in Fig. 18A-B, only a very small percentage of the generated routes have a relative travel time and/or length deviation greater than 1.5 (3.4% for travel time, 4.4% for length). Hence, since there are route observations with relative cost deviations close to 1.5 and thus the estimated bound parameters are close to 1.5, only a small percentage of routes generated are defined as unrealistic by the bounded models and consequently assigned zero choice probabilities / path size contributions eliminated. This restricts how effective the bounded models are at improving upon the fit of their limit models. The bounded models are however more robust (than the non-bounded models) to changes in the adopted choice sets. If the choice sets are expanded, all routes generated with a relative cost deviation greater than 1.5 will have no effect upon the estimation and resultant choice probabilities of the bounded models. The non-bounded models will however all be affected, and some potentially quite significantly (e.g. MNL, PSL). Generating routes with a relative cost deviation less than 1.5 will though affect the bounded models. This means though that either the choice sets were mis-generated initially, outlier observations have resulted in a large estimated bound, or the universal bound mis-represents actual OD-specific relative cost bounds, or all of these. Obtaining multiple route choice observations from the OD movements and estimating OD-specific bounds would lead to far more accurate estimated bounded models, and far greater goodness-of-fit improvements over the limit models. Moreover, it would improve robustness to the adopted choice sets.

To demonstrate how the bounded models can be more effective at improving the fit of their limit models, we re-estimate the models after removing a further 872 route observations from the data set where either the relative travel time or length deviation is over 1.2, leaving 7151 observations. This means that there are now 30.4% and 27.4% of the generated routes that have a relative travel time and length deviation, respectively, greater than the expected estimated bound of 1.2 (as opposed to previously 3.4% and 4.4% for 1.5). Hence, with more routes within the choice sets judged as being unrealistic, the negative effects of not excluding these from route choice should be greater. Table 11 shows the estimated parameters and Log-Likelihood values for the re-estimated models, as well as the penalised-likelihood criteria. As expected, the estimated bound parameters are approximately 1.2, apart from for the BBPS model where the estimate is very large, again approximating $\varphi \to \infty$ and the GPSL$'$ model. As shown, the BCM, and BBPS$_{(\lambda=\theta)}$ & BAPS models now all improve significantly more upon the fit of their limit models MNL, GPSL$'_{(\lambda=\theta)}$, and APSL, respectively.

As noted above, when 82 of the most costly observations are removed from the full data set and the GPSL model is re-estimated, the travel cost parameters increase slightly not having to provide fit for the costly observations, and the $\lambda$ parameter becomes slightly larger to counterbalance within the contribution factors. As can be seen from Table 11 after removing a further 872 costly observations, the GPSL travel cost parameters increase significantly and hence the $\lambda$ parameter increases dramatically too, supporting the trend.

| | $\hat{\alpha}_1$ | $\hat{\alpha}_2$ | $\hat{\beta}$ | $\hat{\lambda}$ | $\hat{\varphi}$ | $LL$ | AIC | BIC | CAIC |
|---|---|---|---|---|---|---|---|---|---|
| MNL | 1.066 | 1.161 | | | | -15159 | 30322 | 30336 | 30337 |
| PSL | 1.231 | 1.079 | 1.149 | | | -14883 | 29772 | 29793 | 29796 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| GPSL | 0.621 | 0.477 | 0.811 | 203.43 | | -13254 | 26516 | 26544 | 26548 |
| GPSL$'$ | 0.633 | 0.519 | 0.696 | 10.962 | | -13301 | 26610 | 26638 | 26642 |
| GPSL$'_{(\lambda=\theta)}$ | 0.832 | 0.589 | 1.548 | | | -14146 | 28298 | 28319 | 28322 |
| APSL | 0.792 | 0.606 | 0.825 | | | -13771 | 27548 | 27569 | 27572 |
| BCM | 0.973 | 1.049 | | | 1.194 | -15050 | 30106 | 30127 | 30130 |
| BBPS$_{(\lambda=\theta)}$ | 0.731 | 0.481 | 1.631 | | 1.197 | -13960 | 27928 | 27956 | 27960 |
| BBPS | 0.633 | 0.519 | 0.696 | 10.962 | 3.940 | -13301 | 26612 | 26646 | 26651 |
| BAPS | 0.681 | 0.505 | 0.838 | | 1.201 | -13582 | 27172 | 27199 | 27204 |

**Table 11.** Real-life case-study: Re-estimation results after removing observations with relative travel time or length deviations greater than 1.2, and penalised-likelihood criteria.

## 8 Conclusion

This paper develops a new route choice modelling framework that deals with both route overlap and unrealistic routes in a theoretically consistent, robust, and mathematically well-defined way, and demonstrates its computational feasibility and estimatibility on large-scale networks. Path Size Logit route choice models capture the correlation between routes by including correction terms within the route utility functions. This provides a convenient closed-form solution for implementation in traffic network models. The deficiency of based Path Size Logit (PSL) model, in its sensitivity to unrealistic routes in the adopted choice sets, is well established. By weighting the contributions of routes to path size terms, current PSL model variants (e.g. Generalised PSL (GPSL), alternative GPSL (GPSL$'$), & Adaptive PSL (APSL)) reduce the negative impact the unrealistic routes have upon the correction factors and thus choice probabilities of realistic routes. However, the effectiveness of this technique worsens as the choice sets are expanded and more unrealistic routes are included. In this study we develop a path size choice model that entirely eliminates the path size contributions and undesirable effects of unrealistic routes.

To tackle this, we explored the integration of PSL concepts with the recently developed Bounded Choice Model (BCM). The BCM provides a consistent criterion for determining restricted choice sets of feasible routes and route choice probability, though route correlation is not considered. This paper derives the natural form for a Bounded Path Size (BPS) model whereby path size choice model utilities are inserted into the BCM formula; however, this led to behavioural inconsistencies and/or undesirable mathematical properties, which were demonstrated by a series of examples. Five desirable properties are consequently established for a mathematically well-defined BPS model that utilises a consistent criterion for assigning zero choice probabilities to unrealistic routes while eliminating their path size contributions.

In order to solve these challenges, an alternative form for a BPS model is derived and two models are consequently formulated that adopt this form: the Bounded Bounded Path Size (BBPS) model and Bounded Adaptive Path Size (BAPS) model, which satisfy many of the desired properties, as discussed/demonstrated.

1. The BBPS model has a consistent criterion for assigning zero choice probabilities to unrealistic routes and eliminating path size contributions, but is not internally consistent. The attraction of the BBPS model, however, is that the probability relation is closed-form.
2. The BAPS model has a consistent criterion for assigning zero choice probabilities to unrealistic routes, eliminating the path size contributions of unrealistic routes, and determining route choice probabilities and path size contributions (internally consistent). The BAPS model is, however, not closed-form since the path size contribution factors are based upon choice probability ratios, and hence the probability relation is an implicit function, naturally expressed as a fixed-point problem. Two formulations for the BAPS model are given: one that has a continuous choice probability function but no formal proofs for solution existence and uniqueness, and one modified version that does not have a continuous distribution, but solutions can be proven to exist and be unique, and the proofs are given. The modified version can approximate the standard version to an arbitrary precision (i.e. by setting a very small value for the parameter $\tau$), however, thus approximating continuity, and hence in practice we use the modified formulation with a small value of $\tau$.

This paper proves that choice probability solutions to the BAPS model are guaranteed to exist, and provides conditions under which solutions are unique. These conditions are only sufficient conditions for uniqueness, however, and a method is proposed and demonstrated for estimating the actual uniqueness conditions.

To show that the parameters of the BBPS & BAPS models can be estimated, a Maximum Likelihood Estimation procedure is proposed for estimating the BBPS & BAPS models with tracked route observation data. Application to the Sioux Falls network shows it is generally possible to reproduce assumed true parameters. The BBPS & BAPS models are then estimated using real tracked route GPS data on a large-scale network. Results show that the BBPS$_{(\lambda=\theta)}$ and BAPS models outperform their limit models GPSL$'_{(\lambda=\theta)}$ and APSL, respectively, but that the BBPS model approximates the GPSL$'$ model. This indicates that the GPSL$'$ and GPSL models provide better fits to real data not by design but by capturing something other than the correlation between the realistic routes within the path size terms.

The BAPS model requires a fixed-point algorithm to approximate solutions. The paper assesses the computational performance of the Fixed-Point Iteration Method for calculating choice probabilities and estimating the parameters of the BAPS model, where accuracy is compared with computation time. Results indicate that accurate choice probability solutions and parameter estimates can be obtained by feasible computation times. It is also shown that BAPS model choice probability computation times can be quicker than for APSL, due to its implicit restriction of choice sets to having fewer routes.

The theory suggests that the BAPS model is more behaviourally realistic than the BBPS model, which is supported by the estimation results, and thus our recommendation is that the BAPS model is used where it is computationally feasible to do so. The BBPS model offers a more computationally practical alternative.

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# 10 Appendix

## 10.1 Appendix A – Derivation of the Bounded Choice Model

First, we define the pdf's and cdf's of relevant probability distributions. The pdf of a Gumbel distribution with mode $\zeta$ and scale $\theta^{-1}$ ($\theta > 0$) is:

$$f_G(x;\zeta,\theta) = \theta \exp\left(-\left(\theta(x-\zeta) + \exp\left(-\theta(x-\zeta)\right)\right)\right), \qquad (-\infty < x < \infty),$$

and the cdf is:

$$F_G(x;\zeta,\theta) = \exp\left(-\exp\left(-\theta(x-\alpha)\right)\right), \qquad (-\infty < x < \infty).$$

Supposing that $\epsilon_1$ and $\epsilon_2$ are individually and identically distributed Gumbel random variables, the difference random variable $\varepsilon = \epsilon_1 - \epsilon_2$ is a logistic distribution with pdf (for mean $\mu$ and scale $\theta^{-1}$) equal to:

$$f_L(x;\mu,\theta) = \theta \exp\big(-\theta(x-\mu)\big)\big(1+\exp\big(-\theta(x-\mu)\big)\big)^{-2}, \qquad (-\infty < x < \infty),$$

and cdf:

$$F_L(x;\mu,\theta) = \big(1+\exp\big(-\theta(x-\mu)\big)\big)^{-1}, \qquad (-\infty < x < \infty).$$

If $\epsilon_1$ and $\epsilon_2$ have mode 0 and scale $\theta^{-1}$ it follows that $\varepsilon$ has mean 0 and scale $\theta^{-1}$.

The BCM proposes that each route $i \in R$ is compared with an imaginary reference alternative $r^*$ in terms of difference in random utility, and imposes a bound, $\psi$, upon this random utility difference. In this study, the reference alternative is the route with the best utility. If $U_i$ and $V_i$ are the random and deterministic utilities for route $i \in R$, respectively, the difference in random utility relative to the reference alternative for route $i \in R$ is:

$$U_{r^*} - U_i = V_{r^*} + \epsilon_{r^*} - V_i - \epsilon_i = \max(V_l : l \in R) - V_i + \epsilon_{r^*} - \epsilon_i = \max(V_l : l \in R) - V_i + \varepsilon_i,$$

where $\epsilon_i$ is the individually and identically distributed random variable error term for route $i \in R$, and $\varepsilon_i$ is the difference random variable for route $i \in R$ with the reference alternative. The MNL model can be derived by assuming the $\epsilon_i$ error terms are Gumbel distributed and thus the $\varepsilon_i$ difference random error terms assume the logistic distribution. The BCM, however, proposes that the difference random variable error terms $\varepsilon_i$ assume a truncated logistic distribution, obtained by left-truncating a logistic distribution with mean 0 and scale $\theta^{-1}$ at a lower bound of $-\psi$ for some $\psi \geq 0$. Each of these variables thus has pdf:

$$f_T(x;\mu,\theta,\psi) = \begin{cases} 0 & -\infty < x < -\psi \\ \dfrac{f_L(x;\mu,\theta)}{1-F_L(-\psi;\mu,\theta)} & x \geq -\psi \end{cases},$$

and cdf:

$$F_T(x;\mu,\theta,\psi) = \begin{cases} 0 & -\infty < x < -\psi \\ \dfrac{F_L(x;\mu,\theta) - F_L(-\psi;\mu,\theta)}{1-F_L(-\psi;\mu,\theta)} & x \geq -\psi \end{cases}.$$

The probability of choosing route $i \in R$ versus the reference alternative is therefore:

$$\begin{aligned} &\Pr(\text{choosing } i \text{ from } \{i,r^*\}) = \Pr(U_i \geq U_{r^*}) = \Pr(U_{r^*} - U_i \leq 0) \\ &= \Pr(\max(V_l : l \in R) - V_i + \varepsilon_i \leq 0) = \Pr(\varepsilon_i \leq V_i - \max(V_l : l \in R)) \\ &= F_T(V_i - \max(V_l : l \in R)\,; 0,\theta,\psi) \\ &= \begin{cases} 0 & -\infty < V_i - \max(V_l : l \in R) < -\psi \\ \dfrac{F_L(V_i - \max(V_l : l \in R)\,; 0,\theta) - F_L(-\psi;0,\theta)}{1-F_L(-\psi;0,\theta)} & V_i - \max(V_l : l \in R) \geq -\psi \end{cases}, \\ &= \begin{cases} 0 & -\infty < V_i - \max(V_l : l \in R) < -\psi \\ \dfrac{\big(1+\exp\big(-\theta(V_i - \max(V_l : l \in R))\big)\big)^{-1} - (1+\exp(\theta\psi))^{-1}}{1-(1+\exp(\theta\psi))^{-1}} & V_i - \max(V_l : l \in R) \geq -\psi \end{cases}. \end{aligned}$$

The odds ratio for route $i \in R$ versus the reference alternative $r^* \in R$ is then:

$$\eta_i = \frac{\Pr(\text{choosing } i \text{ from } \{i,r^*\})}{1-\Pr(\text{choosing } i \text{ from } \{i,r^*\})} = \frac{F_T(V_i - \max(V_l : l \in R)\,; 0,\theta,\psi)}{1-F_T(V_i - \max(V_l : l \in R)\,; 0,\theta,\psi)}.$$

For $V_i - \max(V_l : l \in R) \geq -\psi$, $\eta_i$ can be re-arranged as follows:

$$\frac{\dfrac{\dfrac{1}{\big(1+\exp\big(-\theta(V_i - \max(V_l : l \in R))\big)\big)} - \dfrac{1}{(1+\exp(\theta\psi))}}{\dfrac{1}{1} - \dfrac{1}{(1+\exp(\theta\psi))}}}{1 - \dfrac{\dfrac{1}{\big(1+\exp\big(-\theta(V_i - \max(V_l : l \in R))\big)\big)} - \dfrac{1}{(1+\exp(\theta\psi))}}{\dfrac{1}{1} - \dfrac{1}{(1+\exp(\theta\psi))}}}$$

$$= \frac{\dfrac{\dfrac{\exp(\theta\psi) - \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)}{\left(1 + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)(1 + \exp(\theta\psi))}}{\dfrac{\exp(\theta\psi)}{(1 + \exp(\theta\psi))}}}{1 - \dfrac{\dfrac{\exp(\theta\psi) - \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)}{\left(1 + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)(1 + \exp(\theta\psi))}}{\dfrac{\exp(\theta\psi)}{(1 + \exp(\theta\psi))}}}$$

$$= \frac{\dfrac{\left(\exp(\theta\psi) - \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)}{\left(1 + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)\exp(\theta\psi)}}{\dfrac{1}{1} - \dfrac{\left(\exp(\theta\psi) - \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)}{\left(1 + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)\exp(\theta\psi)}}$$

$$= \frac{\dfrac{\left(\exp(\theta\psi) - \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)}{\left(1 + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)\exp(\theta\psi)}}{\dfrac{\exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\exp(\theta\psi) + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)}{\left(1 + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\right)\exp(\theta\psi)}}$$

$$= \frac{\exp(\theta\psi) - \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)}{\exp\left(-\theta(V_i - \max(V_l: l \in R))\right)\exp(\theta\psi) + \exp\left(-\theta(V_i - \max(V_l: l \in R))\right)}$$

$$= \frac{\exp(\theta\psi)\exp\left(\theta(V_i - \max(V_l: l \in R))\right) - 1}{\exp(\theta\psi) + 1}$$

$$= \frac{\exp\left(\theta(V_i - \max(V_l: l \in R) + \psi)\right) - 1}{\exp(\theta\psi) + 1}.$$

Thus, given the above re-arranging, the odds ratio $\eta_i$ for route $i \in R$ versus the reference alternative $r^* \in R$ is:

$$\eta_i = \begin{cases} 0 & -\infty < V_i - \max(V_l: l \in R) < -\psi \\ \dfrac{\exp\left(\theta(V_i - \max(V_l: l \in R) + \psi)\right) - 1}{\exp(\theta\psi) + 1} & V_i - \max(V_l: l \in R) \geq -\psi \end{cases},$$

which can be written succinctly as:

$$\eta_i = \frac{\left(\exp\left(\theta(V_i - \max(V_l: l \in R) + \psi)\right) - 1\right)_+}{\exp(\theta\psi) + 1},$$

where $(\cdot)_+ = \max(0, \cdot)$.

Now, due to the Independence from Irrelevant Alternatives (IIA) property, the probability ratio between any two routes $i, j \in R$ where $P_i > 0$ and $P_j > 0$ is the ratio of the odds ratios:

$$\frac{P_i}{P_j} = \frac{\eta_i}{\eta_j} = \frac{\dfrac{\Pr(\text{choosing } i \text{ from } \{i, r^*\})}{1 - \Pr(\text{choosing } i \text{ from } \{i, r^*\})}}{\dfrac{\Pr(\text{choosing } j \text{ from } \{j, r^*\})}{1 - \Pr(\text{choosing } j \text{ from } \{j, r^*\})}}$$

$$= \frac{\left(\exp\left(\theta(V_i - \max(V_l: l \in R) + \psi)\right) - 1\right)_+}{\left(\exp\left(\theta\left(V_j - \max(V_l: l \in R) + \psi\right)\right) - 1\right)_+}.$$

Thence, since the non-zero probabilities must add up to 1, the BCM probability for route $i \in R$ is:

$$P_i = \frac{\left(\exp\left(\theta(V_i - \max(V_l: l \in R) + \psi)\right) - 1\right)_+}{\sum_{j \in R}\left(\exp\left(\theta\left(V_j - \max(V_l: l \in R) + \psi\right)\right) - 1\right)_+}.$$

Finally, setting $\psi = (1 - \varphi)\max(V_l: l \in R)$:

$$P_i = \frac{\left(\exp\left(-\theta(V_i - \varphi\max(V_l: l \in R))\right)\right)_+}{\sum_{j \in R}\left(\exp\left(-\theta\left(V_j - \varphi\max(V_l: l \in R)\right)\right)\right)_+}.$$

## 10.2 Appendix B – Derivation of Proposed BPS Model Form

Suppose the probability of choosing route $i \in R$ relates as:

$$P_i = Q_i^1 \times Q_i^2 \times \chi,$$

where

$$Q_i^1 = \frac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l : l \in R))\right) - 1\right)_+}{\sum_{j \in R}\left(\exp\left(-\theta\left(c_j - \varphi \min(c_l : l \in R)\right)\right) - 1\right)_+}, \qquad Q_i^2 = \frac{e^{\beta \ln(\gamma_i)}}{\sum_{j \in R} e^{\beta \ln(\gamma_j)}},$$

and $\chi$ is a normalisation constant. The probabilities for all routes $r \in R$ must add up to 1:

$$\sum_{r \in R} P_r = \sum_{r \in R} Q_r^1 \times Q_r^2 \times \chi = \left(\sum_{r \in R} \frac{\left(\exp\left(-\theta(c_r - \varphi \min(c_l : l \in R))\right) - 1\right)_+ e^{\beta \ln(\gamma_r)}}{\sum_{j \in R}\left(\exp\left(-\theta\left(c_j - \varphi \min(c_l : l \in R)\right)\right) - 1\right)_+ \sum_{j \in R} e^{\beta \ln(\gamma_j)}}\right) \times \chi = \left(\sum_{r \in R} \frac{X_r}{L}\right) \times \chi = 1,$$

where to simplify notation:

$$X_r = \left(\exp\left(-\theta(c_r - \varphi \min(c_l : l \in R))\right) - 1\right)_+ e^{\beta \ln(\gamma_r)},$$

and

$$L = \sum\nolimits_{j \in R}\left(\exp\left(-\theta\left(c_j - \varphi \min(c_l : l \in R)\right)\right) - 1\right)_+ \sum\nolimits_{j \in R} e^{\beta \ln(\gamma_j)}.$$

By rearranging, the normalisation constant $\chi$ is thus:

$$\chi = \left(\sum_{r \in R} \frac{X_r}{L}\right)^{-1}.$$

Substituting $\chi$ back into the probability relation for route $i \in R$:

$$P_i = Q_i^1 \times Q_i^2 \times \chi = \frac{X_i}{L} \times \left(\sum_{r \in R} \frac{X_r}{L}\right)^{-1} = \frac{X_i}{L} \times \left(\frac{1}{L}\sum_{r \in R} X_r\right)^{-1} = \frac{X_i}{L} \times \frac{L}{\sum_{r \in R} X_r} = \frac{X_i}{\sum_{r \in R} X_r}$$

$$= \frac{\left(\exp\left(-\theta(c_i - \varphi \min(c_l : l \in R))\right) - 1\right)_+ \cdot e^{\beta \ln(\gamma_i)}}{\sum_{r \in R}\left(\exp\left(-\theta(c_r - \varphi \min(c_l : l \in R))\right) - 1\right)_+ \cdot e^{\beta \ln(\gamma_r)}}.$$

## 10.3 Appendix C – Desired Properties for a Bounded Path Size Model

In this section, we establish desired properties for a BPS model by exploring different options for the path size terms for the natural BPS model form in (5).

### 10.3.1 Option 1

Suppose that the path size term for route $i \in R$ is defined as follows:

$$\gamma_i^1 = \sum\nolimits_{a \in A_i} \frac{t_a}{c_i} \frac{1}{\sum_{k \in R} \delta_{a,k}}. \tag{26}$$

The option 1 path size term, $\gamma_i^1$, is equivalent to the PSL path size term. As (26) shows, all routes in the choice set contribute equally to path size terms, however unattractive, and thus unrealistic routes (with zero choice probabilities) negatively impact the choice probabilities of realistic routes (with non-zero choice probabilities) if links are shared. To demonstrate this, consider example network 4 in Fig. 25A where there are 3 routes: Routes 2&3 have travel cost 1 and Route 1 has travel cost $0.5 + \upsilon$, Routes 1&2 are correlated while Route 3 is distinct. Fig. 25B displays the example network 4 option 1 BPS model route choice probabilities as $\upsilon$ is increased from 0.5 to 3, $\theta = \beta = 1$, $\varphi = 2.5$. For $\upsilon = 0.5$, Routes 1&2 have the same unshared travel cost and are thus considered equally attractive. As $\upsilon$ is increased, Route 1 increases in travel cost and decreases in utility. As the utility of Route 1 becomes 2.5 times smaller than the utility of Route 3 (the best alternative), Route 1 attains zero choice probability, but continues to contribute to the path size term of Route 2, which is not desired.

We thus establish the following desired property for a BPS model:

**Desired Property 1 – Consistent Definitions of Unrealistic Routes:** *Routes defined as unrealistic by the choice model (assigned zero choice probabilities) should have zero path size contributions, and vice versa.*

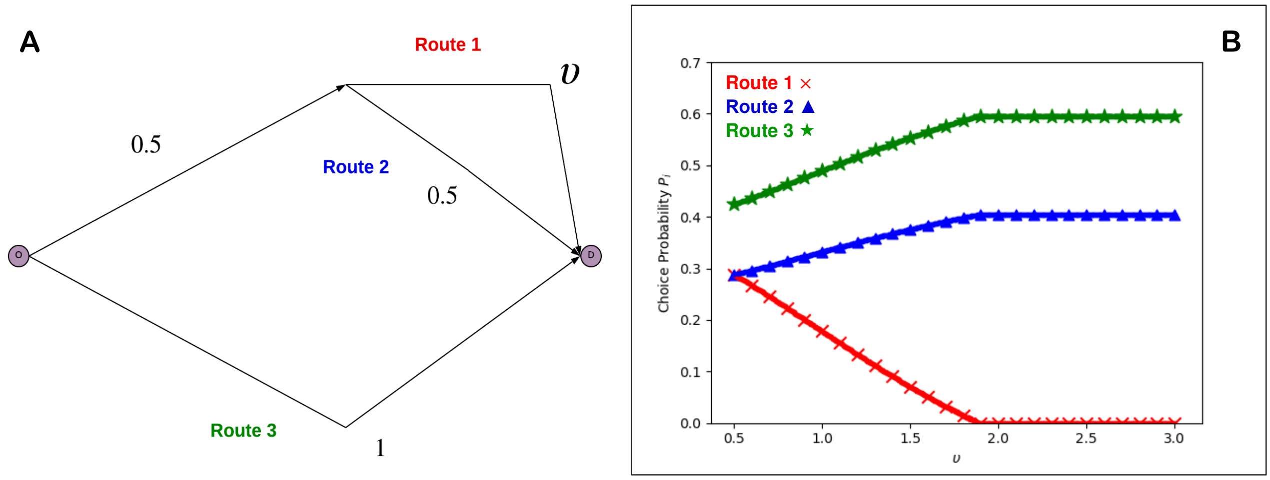



**Fig. 25.** A: Example network 4. B: Example network 4: Option 1 BPS model route choice probabilities for increasing $\upsilon$ ($\theta = \beta = 1$, $\varphi = 2.5$).

### 10.3.2 Options 2&3

Option 1 clarifies that routes defined as unrealistic by the path size terms should have no path size contributions. We explore in options 2&3 below how this might be achieved. However, there is a practical issue for both options that complicates matters. Allowing path size contributions to be zero means that: a) scenarios of $\frac{0}{0}$ can occur within the path size terms; and, b) path size terms can equal zero which consequently results in occurrences of $\ln(0)$ within the route utilities. The $\ln(0)$ issue can be circumvented by negligibly perturbing path size terms that equal zero (by $0 < \tau \ll 1$ say), so that the utility of route $i \in R$ is $V_i = -\theta c_i + \beta \ln((\gamma_i - \tau)_+ + \tau)$. $\ln(0)$ within a route utility implies that that the route is infinitely unattractive, and hence it can be concluded that the route is outside the bound and assigned zero choice probability. A suitably low value for $\tau$ will ensure utilities with zero path size terms are finite but small enough to violate the bound, and for the demonstrations below we set $\tau = 10^{-16}$. The $\frac{0}{0}$ issue, however, cannot be completely circumvented. In order to use options 2&3, one must specify how the path size terms deal with $\frac{0}{0}$, and with each option there is no single formulation that ensures continuity, as we will show. Nevertheless, we present here their formulations as simply as possible for pedagogical purposes only.

#### *10.3.2.1 Option 2*

Suppose that the path size term for route $i \in R$ is defined as follows:

$$\gamma_i^2 = \sum_{a \in A_i} \frac{t_a}{c_i} \frac{(h_i(-\theta \boldsymbol{c}; \omega) - 1)_+}{\sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k}}, \tag{27}$$

where $h_i(-\theta \boldsymbol{c}; \omega) = \exp(-\theta c_i - \omega \max(-\theta c_l : l \in R)) = \exp\big(-\theta(c_i - \omega \min(c_l : l \in R))\big)$, and $\omega > 1$ is the path size contribution bound parameter. Option 2 supposes that routes only contribute to path size terms if they have a cost less than $\omega$ times the cost on the cheapest route, and the path size contribution factors consider ratios of the odds that routes are within this path size contribution bound. As (27) shows, route $k$ only contributes to path size terms if $c_k < \omega \min(c_l : l \in R)$, and as the cost of a route decreases below the contribution bound its path size contribution increases.

Option 2 has two main failings. The first main failing is the practical issue discussed above. If no routes using link $a$ have a cost within the contribution bound, then $\sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k} = 0$ and $\frac{0}{0}$ occurs. Furthermore, if route $i$ has a cost above the contribution bound (i.e. $(h_i(-\theta \boldsymbol{c}; \omega) - 1)_+ = 0$) but for all links in route $i$ at least one route has a cost within the contribution bound (i.e. $\sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k} > 0$, $\forall a \in A_i$), then $\gamma_i^2 = 0$ and $\ln(0)$ occurs in $V_i$. In order to use option 2, one must specify how $\gamma_i^2$ is formulated for $\sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k} = 0$ (to avoid occurrences of $\frac{0}{0}$). There are three alternative formulations for $\gamma_i^2$:

$$\gamma_i^2 = \sum_{a \in A_i} \frac{t_a}{c_i} \times \begin{cases} \dfrac{(h_i(-\theta \boldsymbol{c}; \omega) - 1)_+}{\sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k}} & if \sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k} > 0 \\ Y & if \sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k} = 0 \end{cases},$$

where $Y$ has three alternative values, equal to either 0, 1, or $\frac{1}{\sum_{k \in R} \delta_{a,k}}$, depending on how $\frac{(h_i(-\theta \boldsymbol{c}; \omega) - 1)_+}{\sum_{k \in R} (h_k(-\theta \boldsymbol{c}; \omega) - 1)_+ \delta_{a,k}} \to \frac{0}{0}$.

The second main failing is that the model is internally inconsistent with how routes are defined as being (un)realistic. The natural BPS model probability relation in (5) bounds the route utilities so that routes with a relatively unattractive combination of travel cost and distinctiveness are assigned zero choice probabilities. The option 2 path size terms, however, define a route as unrealistic if it has a large travel cost only, and subsequently bound the route costs so that expensive routes have zero path size contributions. The option 2 path size terms thus potentially result in an inconsistent model, as routes with non-zero choice probabilities may have zero path size contributions, and/or vice versa. To demonstrate, consider example network 4 in Fig. 25A. Fig. 26A-B display example network 4 option 2 BPS model choice probabilities for $\omega = 1.5$ and $\omega = 3$, respectively, as $\upsilon$ is increased from 0.5 to 3, $\Upsilon = \theta = \beta = 1$, $\varphi = 2.5$. In Fig. 26A, as the path size contribution bound parameter is more restrictive than the model bound, the path size contribution of Route 1 to Route 2 is eliminated before Route 1 reaches zero choice probability. Conversely in Fig. 26B, as the contribution bound is less restrictive than the model bound, Route 1 reaches zero probability before its contribution to Route 2 is eliminated.

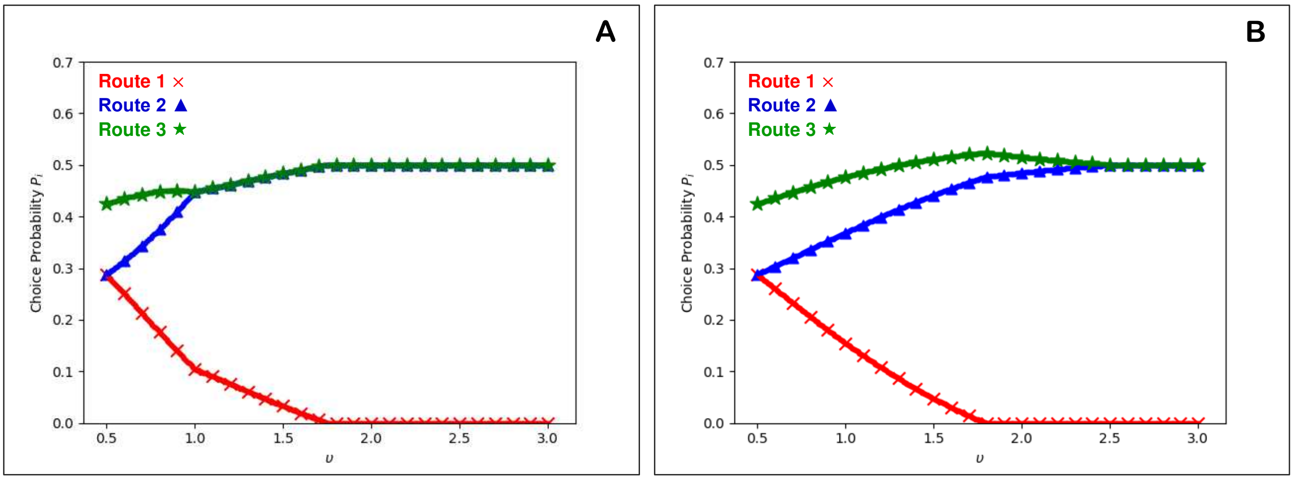
Option 2 also requires the estimation of an additional bound parameter, which makes estimation more difficult, and which can amplify the inconsistency of the model due to the different bound considerations. It is possible that the model bound and path size contribution bound could equate ($\omega = \varphi$), so that routes have zero choice probabilities and/or zero path size contributions if they have a utility/cost $\varphi$ times worse than the best respective route, but there is no real theoretical basis for this. Fig. 26C displays example network 4 option 2 BPS model choice probabilities as $\upsilon$ is increased from 0.5 to 3, with $\omega = \varphi = 2.5$, $\Upsilon = \theta = \beta = 1$. As shown, internal inconsistency still occurs with equated bounds. This does though at least decrease the number of parameters for estimation. The inconsistency of the resultant option 2 model is amplified if the two bound parameters $\varphi$ and $\omega$ have significantly different restrictions on the assessed feasibility of routes, as Fig. 26A-B show. If the model bound $\varphi$ is restrictive so that very few routes have non-zero choice probabilities, but the contribution bound is unrestrictive so that many routes have non-zero path size contributions, or vice versa, then the model is clearly more inconsistent than if the two bound parameters were similarly restricting.

From exploring option 2, we establish the following desired properties for a BPS model:

**Desired Property 2 – Well-Defined Functions:** *The model functions should be well-defined across their domain.*

**Desired Property 3 – Internal Consistency:** *The model should be internally consistent, i.e. there is a consistent assessment of the feasibility of routes between probability relation and path size contribution factors.*

Specifically, Desired Property 2 covers the avoidance of occurrences of $\frac{0}{0}$ in the path size terms / $\ln(0)$ within the route utilities, which occur naturally when routes have zero path size contributions, as shown above and below. It is worth noting that satisfying Desired Property 3 – Internal Consistency is enough to satisfy Desired Property 1 – Consistent Definitions of Unrealistic Routes, but the vice versa is not true, as shown in Section 10.3.3.



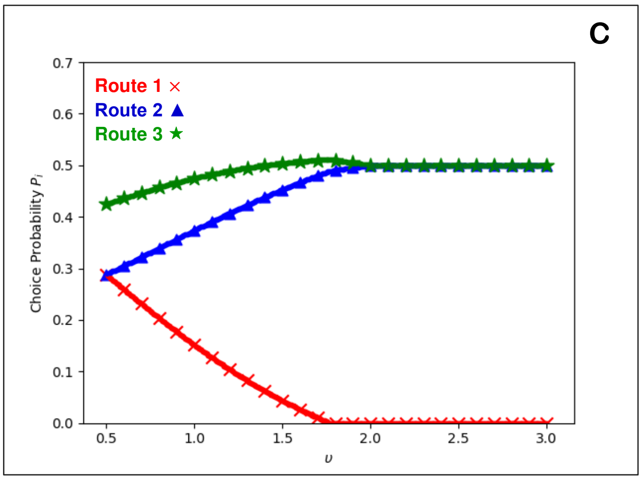



**Fig. 26.** Example network 4: Option 2 BPS model route choice probabilities for increasing $\upsilon$ ($Y = \theta = \beta = 1$, $\varphi = 2.5$). **A:** $\omega = 1.5$. **B:** $\omega = 3$. **C:** $\omega = 2.5$

### *10.3.2.2 Option 3*

Suppose that the path size term for route $i \in R$ is defined as follows:

$$\gamma_i^3(\boldsymbol{P}) = \sum\nolimits_{a \in A_i} \frac{t_a}{c_i} \frac{P_i}{\sum_{k \in R} P_k \delta_{a,k}} = \sum\nolimits_{a \in A_i} \frac{t_a}{c_i} \frac{1}{\sum_{k \in R} \left(\frac{P_k}{P_i}\right) \delta_{a,k}}, \tag{28}$$

where $\boldsymbol{P}$ is a route choice probability vector, and the option 3 BPS model choice probabilities, $\boldsymbol{P}^*$, are a solution to the fixed-point problem $\boldsymbol{P} = \boldsymbol{H}(\boldsymbol{\gamma}^3(\boldsymbol{P}))$ in $D$, where:

$$H_i(\boldsymbol{\gamma}^3(\boldsymbol{P})) = \frac{\left(h_i\left(-\theta \boldsymbol{c} + \beta \ln(\boldsymbol{\gamma}^3(\boldsymbol{P}))\right) - 1\right)_+}{\sum_{j \in R}\left(h_j\left(-\theta \boldsymbol{c} + \beta \ln(\boldsymbol{\gamma}^3(\boldsymbol{P}))\right) - 1\right)_+}, \qquad \forall i \in R.$$

The option 3 path size terms propose that routes contribute according to ratios of choice probability, and thus the resultant model is internally consistent. The probability relation is an implicit function involving the choice probabilities, and solutions to the model are solutions to the fixed-point problem. Whereas the APSL domain for choice probability solutions, $D^{(\tau)}$, does not allow routes to have zero choice probabilities, the option 3 BPS model domain, $D$, does allow for zero probabilities. This is a requirement since the model assigns zero choice probabilities / eliminates the path size contributions of routes with infeasibly low utilities. With this though, $\frac{0}{0}$ occurs in the path size terms when $\sum_{k \in R} P_k \delta_{a,k} = 0$, and $\ln(0)$ occurs in the route utilities when $P_i = 0$ and $\sum_{k \in R; k \neq i} P_k \delta_{a,k} > 0$ for all $a \in A_i$. In order to use option 3. one must specify how $\gamma_i^3$ is formulated for $\sum_{k \in R} P_k \delta_{a,k} = 0$. There are again three alternative formulations for $\gamma_i^3$:

$$\gamma_i^3 = \sum\nolimits_{a \in A_i} \frac{t_a}{c_i} \times \begin{cases} \frac{P_i}{\sum_{k \in R} P_k \delta_{a,k}} & if \sum\nolimits_{k \in R} P_k \delta_{a,k} > 0 \\ Y & if \sum\nolimits_{k \in R} P_k \delta_{a,k} = 0 \end{cases},$$

where $Y$ has three alternative values, equal to either 0, 1, or $\frac{1}{\sum_{k \in R} \delta_{a,k}}$, depending on how $\frac{P_i}{\sum_{k \in R} P_k \delta_{a,k}} \to \frac{0}{0}$.

Option 3 has two other main failings. The first of which is the unconditional non-uniqueness of solutions. The 'active choice set' is the restricted choice set of routes with non-zero choice probabilities. In the case of the option 3 BPS model, there are two types of solution non-uniqueness: *inter-active-choice-set non-uniqueness* and *intra-active-choice-set non-uniqueness*. Intra-active-choice-set non-uniqueness is where there are multiple choice probability solutions within the active choice sets, and inter-active-choice-set non-uniqueness is where there are multiple solutions between active choice sets. Inter-active-choice-set non-uniqueness is much more problematic than intra-active-choice-set non-uniqueness, and having a single active choice set where multiple choice probability solutions exist is more manageable than having multiple active choice sets where solutions exist. If there is just one active choice set where solutions exist, then at least it is known which routes are defined as unrealistic, and it's possible that there will be some conditions under which solutions within the active choice set are unique. However, if it is possible for multiple active choice sets to have solutions, then it is unlikely that uniqueness conditions can be established (conditions under which there is only ever one active choice set with solutions), and an active choice set selection procedure is required.

Inter-active-choice-set non-uniqueness occurs extensively for the option 3 BPS model due to the route utilities not being fixed and the potential for them to vary massively according to the active choice set. Without fixed utilities, the maximum utility route(s) and value can vary, and different routes can have utilities within the bound. To demonstrate, consider example network 5 in Fig. 27 where there are 5 routes; Table 12 gives the route information. As Fig. 27 shows, Routes 1-4 are correlated, and Route 5 is distinct. Using an exhaustive search for active choice set solutions, Table 13, Table 14, & Table 15 display all of the BPS model option 3 choice probability solutions for $Y = 0$, $Y = 1$, and $Y = \frac{1}{\sum_{k\in R}\delta_{a,k}}$, respectively, for $\theta = \beta = 1$, $\varphi = 2$. $\bar{R} \subseteq R$ is the restricted choice set of active routes. There are 17, 3, and 5 active choice sets in which solutions exist for $Y = 0$, $Y = 1$, and $Y = \frac{1}{\sum_{k\in R}\delta_{a,k}}$, respectively. For these parameter settings there is intra-active-choice-set uniqueness. However, to demonstrate how there can also be intra-active-choice-set non-uniqueness, Table 16 displays two BPS model option 3 choice probability solutions for the active choice set $\bar{R} = \{1,2,5\}$, with $Y = 0$, $\theta = 1$, and $\beta = \varphi = 5$.

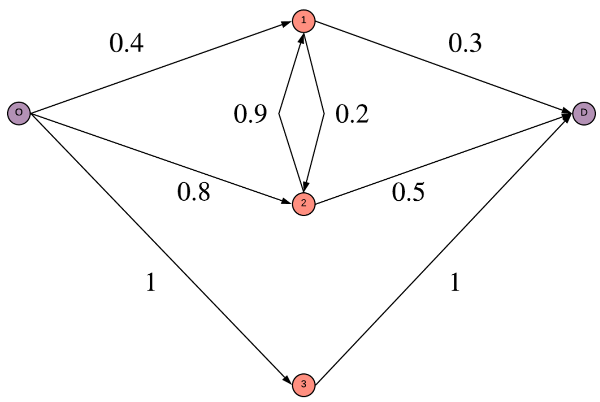



**Fig. 27.** Example network 5.

| Route | Node Traversal | Travel Cost |
|---|---|---|
| 1 | $O \rightarrow 1 \rightarrow D$ | 0.7 |
| 2 | $O \rightarrow 1 \rightarrow 2 \rightarrow D$ | 1.1 |
| 3 | $O \rightarrow 2 \rightarrow 1 \rightarrow D$ | 2 |
| 4 | $O \rightarrow 2 \rightarrow D$ | 1.3 |
| 5 | $O \rightarrow 3 \rightarrow D$ | 2 |

**Table 12.** Example network 5 route information.

| $\bar{R}$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ | $\bar{R}$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| {5} | 0 | 0 | 0 | 0 | 1 | {2,4} | 0 | 0.590 | 0 | 0.410 | 0 |
| {4} | 0 | 0 | 0 | 1 | 0 | {2,4,5} | 0 | 0.498 | 0 | 0.346 | 0.156 |
| {4,5} | 0 | 0 | 0 | 0.765 | 0.235 | {2,3} | 0 | 0.901 | 0.099 | 0 | 0 |
| {3} | 0 | 0 | 1 | 0 | 0 | {2,3,5} | 0 | 0.819 | 0.09 | 0 | 0.09 |
| {3,5} | 0 | 0 | 0.5 | 0 | 0.5 | {2,3,4} | 0 | 0.610 | 0.026 | 0.365 | 0 |
| {3,4} | 0 | 0 | 0.101 | 0.899 | 0 | {2,3,4,5} | 0 | 0.517 | 0.022 | 0.309 | 0.153 |
| {3,4,5} | 0 | 0 | 0.076 | 0.676 | 0.249 | {1} | 1 | 0 | 0 | 0 | 0 |
| {2} | 0 | 1 | 0 | 0 | 0 | {1,4} | 0.906 | 0 | 0 | 0.094 | 0 |
| {2,5} | 0 | 0.901 | 0 | 0 | 0.099 | | | | | | |

**Table 13.** Example network 5: All option 3 BPS model choice probabilities solutions ($Y = 0$, $\theta = \beta = 1$, $\varphi = 2$).

| $\bar{R}$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ |
|---|---|---|---|---|---|
| {2,3,5} | 0 | 0.819 | 0.09 | 0 | 0.09 |
| {2,3,4,5} | 0 | 0.517 | 0.022 | 0.309 | 0.153 |
| {1,4} | 0.906 | 0 | 0 | 0.094 | 0 |

**Table 14.** Example network 5: All option 3 BPS model choice probabilities solutions ($Y = 1$, $\theta = \beta = 1$, $\varphi = 2$).

| $\bar{R}$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ |
|---|---|---|---|---|---|
| {2,5} | 0 | 0.901 | 0 | 0 | 0.099 |
| {2,3,5} | 0 | 0.819 | 0.09 | 0 | 0.09 |

| | | | | | |
|---|---|---|---|---|---|
| {2,3,4,5} | 0 | 0.517 | 0.022 | 0.309 | 0.153 |
| {1} | 1 | 0 | 0 | 0 | 0 |
| {1,4} | 0.906 | 0 | 0 | 0.094 | 0 |

**Table 15.** Example network 5: All option 3 BPS model choice probabilities solutions ($Y = \frac{1}{\sum_{k \in R} \delta_{a,k}}$, $\theta = \beta = 1$, $\varphi = 2$).

| $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_5$ |
|---|---|---|---|---|
| 0.009 | 0.703 | 0 | 0 | 0.288 |
| 0.698 | 0.066 | 0 | 0 | 0.235 |

**Table 16.** Example network 5: Option 3 BPS model choice probabilities solutions for $\bar{R} = \{1,2,5\}$ ($Y = 0$, $\theta = 1$, $\beta = \varphi = 5$).

Another main failing for the option 3 model is that the choice probability function is not always continuous. The option 3 BPS model has trajectories of choice probability solutions as the $\varphi$ bound parameter is varied. For a given trajectory of solutions, as $\varphi$ is decreased, route utilities approach the bound from below resulting in the choice probabilities and thus path size contributions approaching zero. However, since the utilities are not fixed, and are dependent upon $\varphi$, it is possible for the utility of a route to meet the bound (as $\varphi$ is decreased) before its path size contribution to routes meets zero, and as a consequence, the choice probability function is not always continuous in $\varphi$. To demonstrate, consider again example network 5 in Fig. 27. To identify a trajectory of option 3 BPS model solutions for varying $\varphi$ we utilise the following method.

<u>Step 1.</u> Identify a suitably large value for $\varphi$ such that the option 3 BPS model solution will have a non-zero choice probability for all routes.

<u>Step 2.</u> Solve the option 3 BPS model fixed-point problem for this large $\varphi$ with a randomly generated initial condition.

<u>Step 3.</u> Decrement $\varphi$ and obtain the next solution with initial condition set as the solution for the previous $\varphi$.

<u>Step 4.</u> Continue until $\varphi = 1$.

Utilising the above method and plotting the probabilities at each decremented $\varphi$, Fig. 28 displays a trajectory of option 3 BPS model choice probability solutions as $\varphi$ is varied, $Y = \theta = \beta = 1$. As $\varphi$ is decreased, the utility of Route 3 approaches the bound and zero choice probability. However, the utility of Route 3 reaches the bound before the path size contribution of Route 3 to Routes 1&4 reaches zero. Thus, due to the sizeable adjustment of the utilities when Route 3 is removed from the active choice set, the choice probability function is not continuous.

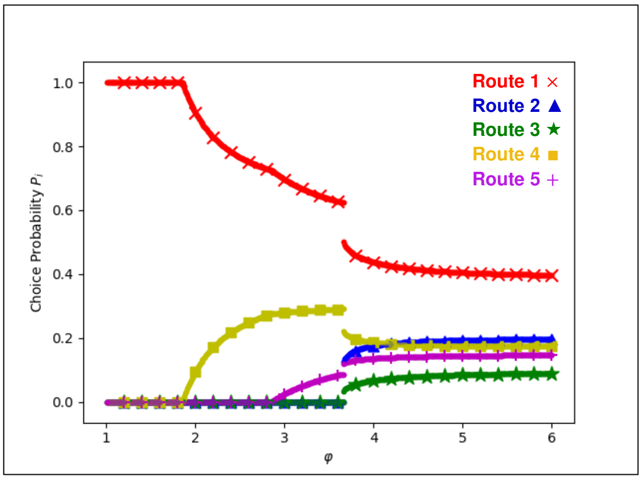



**Fig. 28.** Example network 5: Trajectory of option 3 BPS model choice probability solutions for varying $\varphi$ ($Y = \theta = \beta = 1$)

From exploring option 3, we establish the following desired properties for a BPS model:

**Desired Property 4 – Uniqueness:** *Route choice probability solutions are inter-active-choice-set unique (where there is only one active choice set in which solutions exist), and conditions can be established for intra-active-choice-set uniqueness (where for a given active choice set there is only one solution).*

**Desired Property 5 – Continuity:** *The choice probability function is continuous.*

## 10.4 Appendix D – Existence and Uniqueness of BAPS Model Solutions

In this section we establish a series of theoretical results concerning the BAPS model as defined in (12)-(14), where the guaranteed existence of solutions is proven, and sufficient conditions for the uniqueness of solutions are detailed.

### 10.4.1 Properties

We begin by providing two important properties of the fixed-point function $\boldsymbol{F}$. In Lemma 1 we establish the continuity property of $\boldsymbol{F}$.

**Lemma 1.** $F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ *is a continuous function for* $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$, $\forall i \in R$.

**Proof.** From the definition (14) above it follows that $\overline{\boldsymbol{\gamma}}^{BAPS}$ is continuous in $\boldsymbol{P}$ for all $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$:

$$\lim_{\boldsymbol{P}\to\boldsymbol{P}_0} \overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}) = \overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}_0), \qquad \forall \boldsymbol{P}_0 \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}. \tag{29}$$

If we let $\bar{\Gamma}$ be the set of possible path size terms:

$$\bar{\Gamma} = \left\{\overline{\boldsymbol{\gamma}}^{BAPS} \in \mathbb{R}^{\bar{N}}_{>0} : 0 < \bar{\gamma}_i^{BAPS} \leq 1, \forall i \in \bar{R}(\boldsymbol{c};\varphi)\right\},$$

then from definition (13) above it follows that $f_i$ is continuous in $\overline{\boldsymbol{\gamma}}^{BAPS}$ for all $\overline{\boldsymbol{\gamma}}^{BAPS} \in \bar{\Gamma}$:

$$\lim_{\overline{\boldsymbol{\gamma}}^{BAPS}\to\overline{\boldsymbol{\gamma}}_0} f_i(\overline{\boldsymbol{\gamma}}^{BAPS}) = f_i(\overline{\boldsymbol{\gamma}}_0), \qquad \forall \overline{\boldsymbol{\gamma}}_0 \in \bar{\Gamma}, \qquad \forall i \in R. \tag{30}$$

And, from definition (12) above it follows that $F_i$ is continuous in $x$ for all $x \in [0,1]$:

$$\lim_{x\to x_0} F_i(x) = F_i(x_0), \qquad \forall x_0 \in [0,1], \qquad \forall i \in R. \tag{31}$$

It then follows from (29), (30), and (31) that $F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$, as a composition of continuous functions, is itself continuous in $\boldsymbol{P}$ for all $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$:

$$\lim_{\boldsymbol{P}\to\boldsymbol{P}_0} F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right) = F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}_0)\right)\right), \qquad \forall \boldsymbol{P}_0 \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}, \qquad \forall i \in R.$$

■

We now in Lemma 2 show that the domain of $\boldsymbol{F}$ maps to itself.

**Lemma 2.** $\boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ *maps* $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ *into* $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$.

**Proof.** From definition (14) above it follows that the function $\overline{\boldsymbol{\gamma}}^{BAPS}$ maps $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)} \to \bar{\Gamma}$, from definition (13) it follows that the function $\boldsymbol{f}$ maps $\bar{\Gamma} \to D^{(\bar{R}(\boldsymbol{c};\varphi))}$, and, from definition (12) it follows that the function $\boldsymbol{F}$ maps $D^{(\bar{R}(\boldsymbol{c};\varphi))} \to D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$. It thus follows that the composition of the functions $\overline{\boldsymbol{\gamma}}^{BAPS}$, $\boldsymbol{f}$, and $\boldsymbol{F}$, $\boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$, maps $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)} \to D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$.

■

### 10.4.2 Existence of Solutions

Having established some properties regarding the BAPS model fixed-point function $\boldsymbol{F}$, we consider the existence of BAPS model solutions.

**Proposition 1.** *At least one BAPS model fixed-point solution,* $\boldsymbol{P}^*$*, to the system* $\boldsymbol{P} = \boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ *is guaranteed to exist in* $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$.

**Proof.** $\boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ is a continuous function by Lemma 1, which maps $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ into $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ by Lemma 2, and thus since $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ is a compact convex set, and by Brouwer's Fixed-Point Theorem at least one fixed-point solution, $\boldsymbol{P}^*$, is guaranteed to exist for the system $\boldsymbol{P} = \boldsymbol{F}\left(\boldsymbol{f}\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)$ in $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$.

■

### 10.4.3 Uniqueness of Solutions

Having proven that BAPS model solutions are guaranteed to exist, the next question is whether sufficient conditions exist which ensure BAPS model solutions are unique. In order to do this, we must first establish two key properties of $J_{\boldsymbol{F}}(\boldsymbol{P};\beta)$ which is the Jacobian matrix of first partial derivatives of $\boldsymbol{F}$ evaluated at $\boldsymbol{P}$ and $\beta$.

**Lemma 3.** *The maximum Jacobian matrix norm of* $\boldsymbol{F}\big(\boldsymbol{f}(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});\beta)\big)$ *for all* $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ *at* $\beta = 0$ *is equal to zero:* $\max\big(\|J_{\boldsymbol{F}}(\boldsymbol{P};0)\| : \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\big) = 0$.

**Proof.** From definitions (12) and (13) above it follows that:

$$F_i\big(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});0)\big) =$$

$$\begin{cases} \tau + (1-\bar{N}\tau)\cdot\left(\dfrac{\big(\exp\big(-\theta(c_i - \varphi\min(c_l : l \in R))\big)-1\big)}{\sum_{j\in\bar{R}(\boldsymbol{c};\varphi)}\Big(\exp\Big(-\theta\big(c_j - \varphi\min(c_l : l\in R)\big)\Big)-1\Big)}\right) & if\ i \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & if\ i \notin \bar{R}(\boldsymbol{c};\varphi) \end{cases}, \qquad \forall i \in R. \tag{32}$$

It then follows from (32) that:

$$\frac{\partial F_i\big(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});0)\big)}{\partial P_l} = 0, \qquad \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}, \qquad \forall i,l \in R. \tag{33}$$

It thus follows from (33) that $\|J_{\boldsymbol{F}}(\boldsymbol{P};0)\| = 0, \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$, and hence $\max\big(\|J_{\boldsymbol{F}}(\boldsymbol{P};0)\| : \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\big) = 0$.

■

**Lemma 4.** *The maximum Jacobian matrix norm of* $\boldsymbol{F}\big(\boldsymbol{f}(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});\beta)\big)$, $\max\big(\|J_{\boldsymbol{F}}(\boldsymbol{P};\beta)\| : \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\big)$, is a continuous function for $\beta \in [0,\infty)$.

**Proof.** It follows from the definitions (12), (13), and (14) above that:

$$\frac{\partial F_i\Big(f_i\big(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\big)\Big)}{\partial P_l} =$$

$$\begin{cases} (1-N\tau)\cdot\left(\dfrac{(h_i(-\theta\boldsymbol{c})-1)\cdot\left(\bar{\gamma}_i^{BAPS}(\boldsymbol{P})\right)^{\beta}}{\sum_{j\in\bar{R}(\boldsymbol{c};\varphi)}\big(h_j(-\theta\boldsymbol{c})-1\big)\cdot\left(\bar{\gamma}_j^{BAPS}(\boldsymbol{P})\right)^{\beta}}\right)\cdot\left(\dfrac{\beta\frac{\partial\bar{\gamma}_i^{BAPS}(\boldsymbol{P})}{\partial P_l}}{\bar{\gamma}_i^{BAPS}(\boldsymbol{P})} - \dfrac{\sum_{j\in\bar{R}(\boldsymbol{c};\varphi)}\beta\big(h_j(-\theta\boldsymbol{c})-1\big)\frac{\partial\bar{\gamma}_j^{BAPS}(\boldsymbol{P})}{\partial P_l}\left(\bar{\gamma}_j^{BAPS}(\boldsymbol{P})\right)^{\beta-1}}{\sum_{j\in\bar{R}(\boldsymbol{c};\varphi)}\big(h_j(-\theta\boldsymbol{c})-1\big)\cdot\left(\bar{\gamma}_j^{BAPS}(\boldsymbol{P})\right)^{\beta}}\right) & if\ i,l \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & otherwise \end{cases}, \tag{34}$$

$$\forall i,l \in R,$$

$$\frac{\partial\bar{\gamma}_i^{BAPS}(\boldsymbol{P})}{\partial P_i} = \sum\nolimits_{a\in A_i}\frac{t_a}{c_i}\left(\frac{\sum_{k\in\bar{R}(\boldsymbol{c};\varphi);k\neq i}P_k\delta_{a,k}}{\left(\sum_{k\in\bar{R}(\boldsymbol{c};\varphi)}P_k\delta_{a,k}\right)^2}\right), \qquad \forall i \in \bar{R}(\boldsymbol{c};\varphi), \tag{35}$$

and,

$$\frac{\partial\bar{\gamma}_i^{BAPS}(\boldsymbol{P})}{\partial P_l} = \begin{cases} -\sum\nolimits_{a\in A_i}\dfrac{t_a}{c_i}\dfrac{P_i\delta_{a,l}}{\left(\sum_{k\in\bar{R}(\boldsymbol{c};\varphi)}P_k\delta_{a,k}\right)^2} & if\ l \in \bar{R}(\boldsymbol{c};\varphi) \\ 0 & if\ l \notin \bar{R}(\boldsymbol{c};\varphi) \end{cases}, \qquad \forall i \in \bar{R}(\boldsymbol{c};\varphi), l \in R, l \neq i. \tag{36}$$

From the definitions (35) and (36) above it follows that $\frac{\partial\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})}{\partial\boldsymbol{P}}$ is continuous in $\boldsymbol{P}$ for all $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$:

$$\lim_{\boldsymbol{P}\to\boldsymbol{P}_0}\frac{\partial\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})}{\partial\boldsymbol{P}} = \frac{\partial\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}_0)}{\partial\boldsymbol{P}}, \qquad \forall \boldsymbol{P}_0 \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}. \tag{37}$$

It then follows from (29) and (37) that $\frac{\partial F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)}{\partial P_l}$ as defined in (30), being a composition of continuous functions, is itself continuous in $\boldsymbol{P}$ for all $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$:

$$\lim_{\boldsymbol{P}\to\boldsymbol{P}_0}\frac{\partial F_i\Big(f_i\big(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\big)\Big)}{\partial P_l} = \frac{\partial F_i\Big(f_i\big(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}_0)\big)\Big)}{\partial P_l}, \qquad \forall \boldsymbol{P}_0 \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}, \qquad \forall i,l \in R.$$

Since $\frac{\partial F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P})\right)\right)}{\partial P_l}$ is a continuous function for $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$, $\forall i,l \in R$, $\frac{\partial F_i\left(f_i\left(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});\beta\right)\right)}{\partial P_l}$ is also a continuous function for $\beta \in [0,\infty)$, $\forall i,l \in R$:

$$\lim_{\beta\to\beta_0}\left(\frac{\partial F_i\big(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});\beta)\big)}{\partial P_l}\right) = \frac{\partial F_i\big(f_i(\overline{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});\beta_0)\big)}{\partial P_l}, \qquad \forall \beta_0 \in [0,\infty), \qquad \forall i,l \in R.$$

Hence, since $\max(\|J_{\boldsymbol{F}}(\boldsymbol{P};\beta)\|: \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)})$ is a composition of continuous functions then it itself is a continuous function for $\beta \in [0,\infty)$:

$$\lim_{\beta \to \beta_0} \left(\max\left(\|J_{\boldsymbol{F}}(\boldsymbol{P};\beta)\|: \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\right)\right) = \max\left(\|J_{\boldsymbol{F}}(\boldsymbol{P};\beta_0)\|: \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\right), \qquad \forall \beta_0 \in [0,\infty).$$

■

These two key properties of $J_{\boldsymbol{F}}(\boldsymbol{P};\beta)$ allow us to establish conditions for the uniqueness of solutions.

**Proposition 2.** *There always exist values of* $b > 0$ *such that when the* $\beta$ *parameter is within the range* $0 \le \beta \le b$*, there are unique BAPS model fixed-point solutions,* $\boldsymbol{P}^*$*, to the system* $\boldsymbol{P} = \boldsymbol{F}\left(\boldsymbol{f}(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P});\beta)\right)$ *in* $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$.

**Proof.** $\boldsymbol{F}$ is a *contraction mapping* on the domain $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ if:

a) $\boldsymbol{F}$ maps $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ into itself, so $\boldsymbol{F}\left(\boldsymbol{f}(\bar{\boldsymbol{\gamma}}^{BAPS}(\boldsymbol{P}_0);\beta)\right) \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}, \forall \boldsymbol{P}_0 \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$, and
b) There exists a constant $0 \le \sigma < 1$ such that:

$$\|J_{\boldsymbol{F}}(\boldsymbol{P};\beta)\| \le \sigma, \qquad \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)},$$

where $J_{\boldsymbol{F}}(\boldsymbol{P};\beta)$ is the Jacobian matrix of first partial derivatives of $\boldsymbol{F}$ evaluated at $\boldsymbol{P}$.

If the link cost vector $\boldsymbol{t}$ is fixed (and thus the route cost vector $\boldsymbol{c}$ is fixed), and $\theta$, $\varphi$ are fixed, then for any given $\beta$, if $\boldsymbol{F}$ is a contraction mapping, then since $D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ is a compact convex set, and by Lemma 1, Lemma 2, and the Contraction Mapping Theorem, $\boldsymbol{F}$ emits a unique fixed-point solution $\boldsymbol{P}^* \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$.

It remains to establish the conditions under which $\boldsymbol{F}$ is a contraction mapping. Since by Lemma 3 the maximum Jacobian matrix norm of $\boldsymbol{F}$ for all $\boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}$ at $\beta = 0$ is equal to zero $\left(\max\left(\|J_{\boldsymbol{F}}(\boldsymbol{P};0)\|: \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\right) = 0\right)$, and by Lemma 4 $\max\left(\|J_{\boldsymbol{G}}(\boldsymbol{P};\beta)\|: \forall \boldsymbol{P} \in D^{(\bar{R}(\boldsymbol{c};\varphi),\tau)}\right)$ is a continuous function for $\beta \in [0,\infty)$, then there must always exist values $b > 0$ such that when $\beta$ is within the range $0 \le \beta \le b$ $\boldsymbol{F}$ is a contraction mapping and the sufficient conditions for unique BAPS model solutions are always met.

■

There are cases where the BAPS model has unique solutions for all $\beta > 0$ (i.e. for all values of $b$), for example where all active routes are non-overlapping and the path size terms are consequently all 1 so that $F_i$ collapses to (32), and hence in these cases a maximum value for $b$ does not exist. However, in most cases BAPS model solutions are not unique for all values of $\beta$ and in these cases a maximum value for $b$ exists (denoted $b_{max}$) such that Proposition 2 holds. However, Proposition 2 is only a sufficient condition for unique BAPS model solutions and solutions are not necessarily non-unique for $\beta > b_{max}$. In Section 10.5 below we demonstrate how the true maximum range $0 \le \beta \le \beta_{max}$ for which BAPS model solutions are unique can be estimated.

## 10.5 Appendix E – Satisfying the Desired Properties for a BPS Model

In this section we discuss/demonstrate how the BBPS and BAPS models satisfy the desired properties for a BPS model established in Appendix C.

### 10.5.1 Desired Property 1 – Consistent Definitions of Unrealistic Routes

**Property:** *Routes defined as unrealistic by the choice model (assigned zero choice probabilities) should have zero path size contributions, and vice versa.*

The BBPS and BAPS models both satisfy Desired Property 1 since the proposed BPS model form stipulates that a route has both a zero choice probability and zero path size contributions if and only if it has a travel cost above the bound. This is demonstrated in Section 10.5.3 below.

### 10.5.2 Desired Property 2 – Well-Defined Functions

**Property:** *The model functions should be well-defined across their domain.*

The BBPS and BAPS models both satisfy Desired Property 2, which, specifically, is established so that occurrences of $\frac{0}{0}$ in the path size terms / $\ln(0)$ within the route utilities are avoided. Generally, the path size correction factor for route $i \in R$ is $\kappa_i = \beta \ln(\gamma_i)$, and the path size term of route $i \in R$ is defined as follows:

$$\gamma_i = \sum\nolimits_{a \in A_i} \frac{t_a}{c_i} \frac{W_i}{\sum_{k \in R} W_k \delta_{a,k}},$$

where $W_k$ is the path size contribution weighting of route $k \in R$. If allowing for the weightings to be zero as to eliminate contributions, then $\frac{0}{0}$ occurs when $W_i = \sum_{k \in R} W_k \delta_{a,k} = 0$, and $\gamma_i = 0$ occurs (resulting in $\ln(0)$) when $W_i = 0$ and $\sum_{k \in R; k \neq i} W_k \delta_{a,k} > 0$. Two key features of the proposed BPS model form – of which the BBPS and BAPS model adopt – are that: a) only the realistic routes have path size terms; and, b) the realistic route path size terms only consider the path size contributions of other realistic routes. These two features ensure that the proposed BPS model form has well-defined functions. The form stipulates that the realistic routes are those which have a travel cost less than the bound ($\varphi$ times the cost on the cheapest route), and that the path size contribution weightings of these routes are non-zero. The proposed BPS model path size term definition in (7) thus only considers the path size contribution weightings of routes $k \in R$ that have costs below the bound (routes $k \in \bar{R}(\boldsymbol{c}; \varphi)$), since it is known that these are the realistic routes and have non-zero weightings, and hence occurrences of $\frac{0}{0}$ are avoided. Moreover, since path size terms are only defined for realistic routes where $W_i > 0$, occurrences of $\gamma_i = 0$ and thus $\ln(0)$ are avoided, although (6) precludes occurrences of $\ln(\gamma_i)$ regardless.

### 10.5.3 Desired Property 3 – Internal Consistency

**Property:** *The model should be internally consistent, i.e. there is a consistent assessment of the feasibility of routes for both the probability relation and the path size contribution factors.*

The BAPS model satisfies Desired Property 3 since the BAPS model path size contribution factors assess the feasibility of routes according to their route choice probability, and hence the model is internally consistent. The BBPS model is not internally consistent, however, since the contribution factors assess routes according to their travel cost, with no consideration of distinctiveness, and hence Desired Property 3 is not satisfied.

To demonstrate, consider example network 4 in Fig. 25A. Fig. 29A-B display the example network 4 BBPS model $\lambda = 8$ and BAPS model choice probabilities, respectively, as $\upsilon$ is increased from 0.5 to 3, $\theta = \beta = 1$, $\varphi = 2.5$. As Fig. 29B shows for the BAPS model, as the travel cost of Route 1 increases, its choice probability and consequently path size contribution to Route 2 decreases. As the cost of Route 1 approaches the bound, Route 1 approaches zero choice probability / path size contribution. When $\upsilon = 2$, the travel cost of Route 1 is exactly 2.5 times the cost on the cheapest routes (Routes 2&3), and hence Route 1 is assigned zero choice probability, and its path size contribution is eliminated. In Fig. 29A, however, for the BBPS model, the large $\lambda$ value accentuates the travel cost differences and the contribution of Route 1 to Route 2 diminishes to zero well before the cost of Route 1 reaches the bound and obtains zero probability.

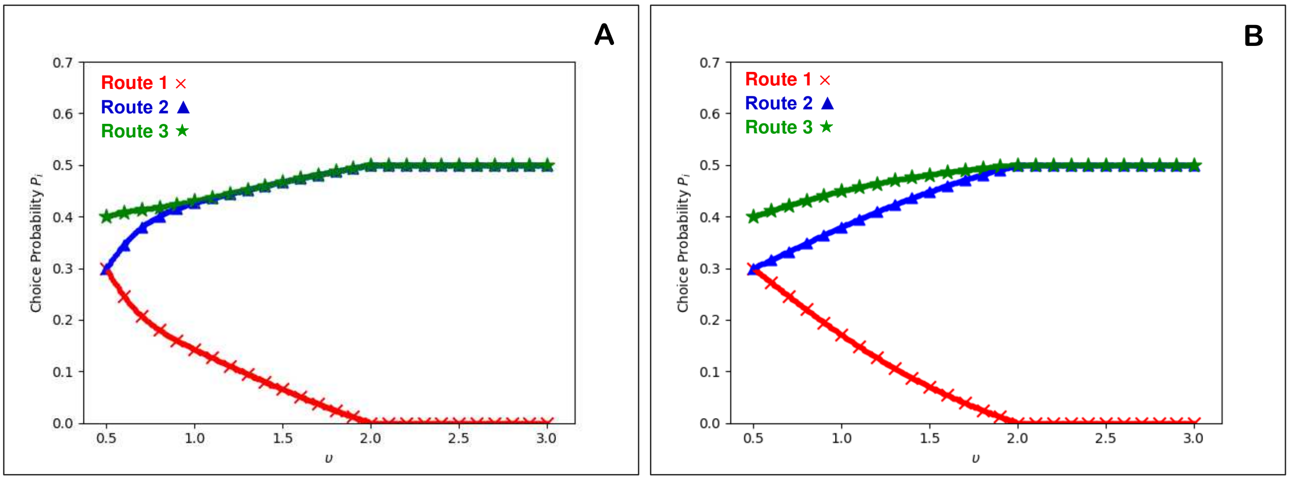



**Fig. 29.** Example network 4: Route choice probabilities for increasing $\upsilon$ ($\theta = \beta = 1$, $\varphi = 2.5$). **A:** BBPS model, $\lambda = 8$. **B:** BAPS model.

### 10.5.4 Desired Property 4 – Uniqueness

**Property:** *Route choice probability solutions are inter-active-choice-set unique (where there is only one active choice set in which solutions exist), and conditions can be established for intra-active-choice-set uniqueness (where for a given active choice set there is only one solution).*

For the proposed BPS model form, there is only one active choice set in which solutions exist: the zero choice probability routes are exactly the routes with travel costs greater than or equal to the bound, and, routes with travel costs below the bound will receive non-zero choice probabilities. This is in contrast to the option 2&3 BPS models in Section 10.1.2 where there are multiple active choice sets in which solutions exist. BBPS & BAPS model choice probability solutions are thus inter-active-choice-set unique, and, since the BBPS model is closed-form, solutions are also intra-active-choice-set unique. BAPS model choice probability solutions are however not intra-active-choice-set unique, though conditions exist under which solutions are.

Duncan et al (2020) demonstrate how APSL choice probability solutions are unique for $\beta$ in the range $0 \leq \beta \leq \beta_{max}$. A similar range exists for the BAPS model. We shall show here: a) that multiple BAPS model solutions can exist; b) that there is a range $0 \leq \beta \leq \beta_{max}$ for $\beta$ in which solutions are unique; and, c) how $\beta_{max}$ can be estimated. To do this, we utilise the same method to that described in Section 4.4 of Duncan et al (2020) for the APSL model. $\beta_{max}$ is estimated by plotting trajectories of BAPS model solutions for varying $\beta$, and identifying where a unique trajectory of solutions ends and multiple trajectories begin. A simple method for obtaining trajectories of BAPS model solutions is as follows:

Step 1. Identify a suitably large value for $\beta$.

Step 2. Solve the BAPS model fixed-point system for this large $\beta$ with a randomly generated initial condition (see Section 5.2.2).

Step 3. Decrement $\beta$ and obtain the next BAPS model solution with initial condition set as the solution for the previous $\beta$.

Step 4. Continue until $\beta = 0$.

By plotting the choice probabilities at each decremented $\beta$, and repeating this method several times, one can determine where non-unique solution trajectories end and hence estimate $\beta_{max}$. If after several repetitions (with different randomly generated initial conditions) only a single trajectory of solutions is shown, then the initial large $\beta$ value is increased. We illustrate the approach graphically, but there is no need to draw graphs for general networks. One can instead observe the choice probability values, where a finer grained decrement of $\beta$ will provide a more accurate estimation of $\beta_{max}$.

To demonstrate, consider again example network 5 in Fig. 27; Fig. 30A-B display trajectories of BAPS model solutions as the $\beta$ parameter is varied for $\varphi = 7$ and $\varphi = 2.5$, respectively, with $\theta = 1$. $\beta$ was decremented by 0.01, and the initial large $\beta$ values were $\beta = 1.5$ for Fig. 30A and $\beta = 10$ for Fig. 30B. The solution trajectory plotting was repeated until multiple clear trajectories were shown. As shown, there is a unique trajectory of choice probability solutions up until $\beta = \beta_{max}$ where there then becomes multiple trajectories. The estimated $\beta_{max}$ values are 0.97 for Fig. 30A and 4.61 for Fig. 30B.

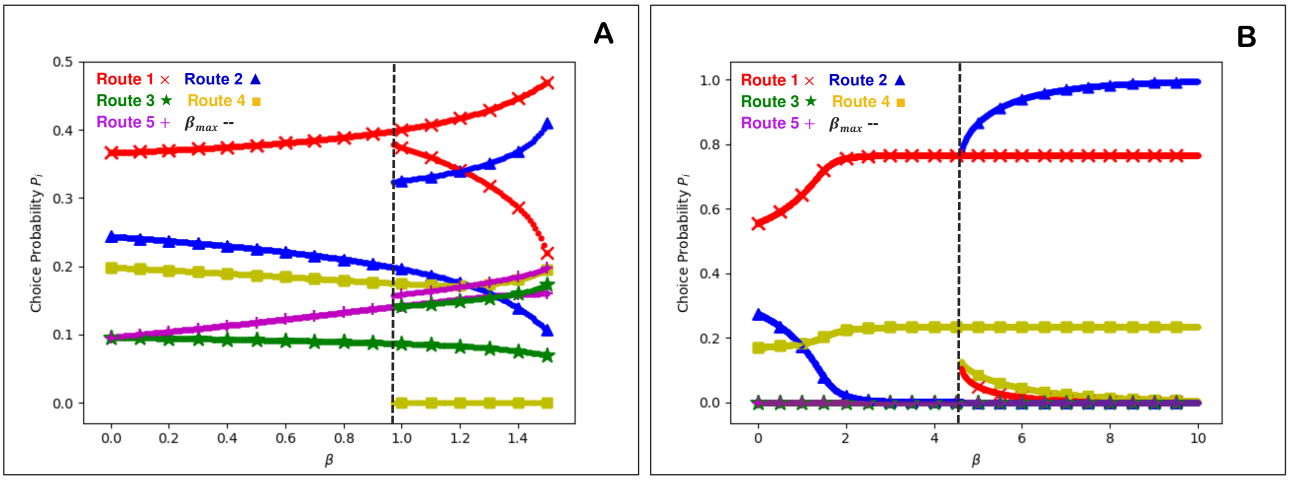



**Fig. 30.** Example network 5: Trajectories of BAPS model choice probability solutions as $\beta$ is varied ($\theta = 1$). **A:** $\varphi = 7$. **B:** $\varphi = 2.5$.

### 10.5.5 Desired Property 5 – Continuity

**Property:** *The choice probability function is continuous.*

The BBPS model has a continuous choice probability function: it is closed-form, and as the cost of a route approaches the bound from below, its choice probability and path size contributions approach zero, and meet exactly at zero. While the modified BAPS model formulation is known to be discontinuous, the standard BAPS model formulation has a continuous choice probability function (if assumed solutions always exist), and the modified version approximates the standard version, thus approximating continuity. Despite having similar path size terms, the standard BAPS model formulation does not suffer from the same discontinuity issue as the option 3 BPS model in Section 10.1. Whereas with the option 3 model the feature that is bounded (route utility) varies as $\varphi$ varies, the feature that is bounded with the BAPS model (route cost) is constant for all $\varphi$. As a consequence, choice probabilities / path size contributions approach zero as routes approach the bound from below, and meet exactly at zero. To demonstrate, consider example network 5 in Fig. 27; Fig. 31A-B display the trajectories of $\text{BBPS}_{(\lambda=0)}$ and BAPS model choice probability solutions, respectively, as $\varphi$ is varied, $\theta = \beta = 1$. As Fig. 31A-B show, as the bound decreases and the route costs approach the bound from below, the choice probabilities approach zero and meet zero at the bound. Since the path size contributions also approach zero as the route costs approach the bound, then there is no adjustment amongst the active route probabilities once a route becomes inactive and hence the choice probability functions are continuous in $\varphi$, and thus travel cost (as shown in Fig. 29).

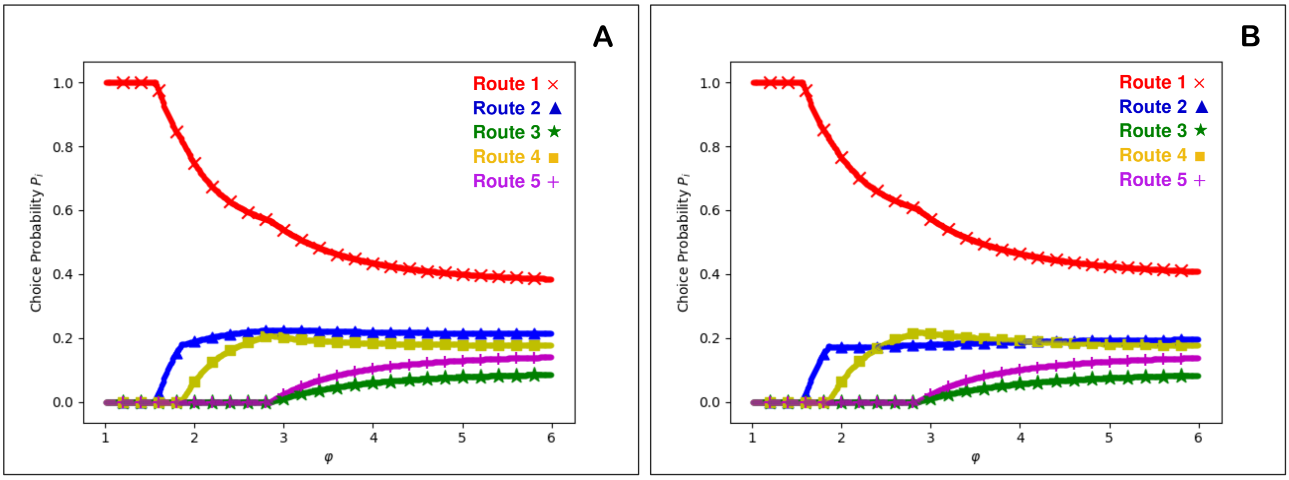



**Fig. 31.** Example network 5: Route choice probabilities for varying $\varphi$ ($\theta = \beta = 1$). **A:** BBPS$_{(\lambda=0)}$ model. **B:** BAPS model.