ALBATROSS – A LEARNING-BASED TRANSPORTATION ORIENTED SIMULATION SYSTEM

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Abstract. This paper describes the conceptual development, operationalization and empirical testing of Albatross: A Learning Based Transportation Oriented Simulation System. This activity-based model of activity-travel behavior is derived from theories of choice heuristics that consumers apply when making decisions in complex environments. The model, one of the most comprehensive of its kind, predicts which activities are conducted when, where, for how long, with whom, and the transport mode involved. In addition, various situational, temporal, spatial, spatial-temporal and institutional constraints are incorporated in the model. The decision tree is proposed as a formalism to represent an exhaustive set of mutual exclusive rules for each decision step in the model. A CHAID decision tree induction method is used to derive decision trees from activity diary data. The case study conducted to develop and test the model indicates that performance of the model is very satisfactory. We conclude therefore that the methodology proposed in this article is useful to develop computational process models of activity-travel choice behavior.

Keywords: activity-based modeling; computational process modeling; decision tree induction; reinforcement learning.

1. INTRODUCTION

The activity based approach in travel demand modeling implies a shift in focus from trips to activities assuming that most travel is not an and in itself but a means to bridge activities that are separated in time and space. The aim of the models is to explain and predict for a given time frame and in an integrated fashion, which activities individuals conduct, where, when, for how long, sometimes with whom, and the transport mode used. The choice of an activity-travel pattern that meets space-time, institutional and household constraints and satisfies as much as possible preferences of the individual, is an inherently complex cognitive task. Acknowledging this complexity, several authors have stressed the importance of understanding the decision making processes that underly activity patterns and proposed computational process models that are consistent with cognitive theories of problem solving, decision making and learning.

The production system is the most influential model of higher-order cognitive processes in cognitive sciences, since it was introduced by Newell and Simon in the early seventies (1972). A production system consists of a set of condition-action rules, called productions, representing long-term memory of the individual and a set of currently active facts or beliefs about a given problem in short term memory. The systems describe

problem solving as a cyclic process of matching productions with items in short-term memory and adding the action of an executed production to short term memory. Because added actions may trigger other productions, the process is repeated until all productions have been tried. The sequence of actions represent steps and the final state of short term memory the outcome of a problem solving process. Think out loud protocols and many experimental findings in the area of memory, learning, and problem solving have been succesfully reproduced in production systems (e.g., Anderson 1983).

As argued by Gärling (1998), this cognitive theory points at forms of imperfect choice behavior not covered by current utility-maximization models based on economic theory. The implications are particularly relevant for activity-based models which consider choices on many facets in interaction. The number of possible activity-travel patterns is the product of all feasible activity sequences and activity profiles. As described by production systems, individuals search a solution space only partially based on heuristics that often yield satisfycing outcomes, but which are not necessarily optimal. The heuristics used determine the sequence in which decisions are made and the choice alternatives and attributes evaluated, and, hence, have impact on outcomes of the process. It is the central argument for computational process models that, even if one is interested in outcomes only, the process by which outcomes are generated need to be represented in activity-based models. Gärling, Kwan and Golledge (1994) comprehensively discuss the theoretical underpinning of these models.

Despite the well-established status of computational process theory, existing attempts to develop computational process models (CPM) are limited. To review work in this field, we make a distinction between a weak and strong definition of CPM. Weak CPM apply a heuristic in the form of some sequential or partially sequential decision making process, but still assume utility-maximiziation or some other form of unbounded rationality at the level of individual decision steps. Regardless whether or not reference is made to theories of heuristic search, several operational activity-based models exist that meet the weak definition. Examples are PCATS (Kitamura and Fujii, 1998), the model system proposed by Bhat (Bhat, 1999), STARCHILD (Recker et al. 1986a, 1986b) and SMASH (Ettema, Borgers and Timmermans, 1993). These models differ in various respects, but have in common that logit models or other forms of algebraic equations are used to predict single-facet choices.

Computational process models that fit the strong definition use a production system or some other rule-based formalism also at the level of individual choice facets. Models that meet this definition are scarce. The best example is *SCHEDULER,* developed by Gärling *et al.* (1989). These authors developed a conceptual framework for understanding the process by which individuals organize their activities (Gärling, 1989, 1992a, 19992b). This framework has been applied to study the possible impact of the introduction of tele-commuting on the activity patterns of commuters (Gärling, Kwan and Golledge, 1994). Only recently, parts of this conceptual model were elaborated and subject of experimental investigation (Gärling, *et al*, 1997, 1998, 1999). Strongly based on this model is GISICAS which uses search heuristics in combination with GIS to generate feasible schedules (Kwan 1997). Another attempt of developing a rule-based model has been reported in Vause (1997), but apparently this work has been discontinued.

This brief summary of the state-of-the-art of computational process models indicates that, to the best of our knowledge, fully operational rule-based models have not been

developed to date. Arguably, the lack of a method of empirically deriving rules of a production system has hampered progress in this field (Golledge *et al.* 1994). Furthermore, the verification of completeness and consistency of production systems presents a problem (Vausse 1997). While being consistent with assumptions of (strong) CPM, the decision tree provides an alternative formalism that has favorable properties in both respects. Methods to induce decision trees from data are available from work in statistics and artificial intelligence. These methods develop a tree by recursively splitting a sample of observations into increasingly homogeneous groups in terms of a given response variable. Decision trees induced in this way describe the data and, at the same time, meet requirements of completeness and consistency.

In this article, we propose a fully operational computational process model based on the decision tree formalism. Albatross, as the model is called, was developed for the Dutch Ministry of Transportation, Public Works and Water Management, to explore possibilities of a rule-based approach and develop a travel demand model for policies impact analysis. This article desribes the conceptual underpinning, operationalization and validation testing of the model. The first section discusses central concepts followed by a description of the proposed approach. An activity-travel diary survey was conducted to collect data for deriving and testing the model. The sections that follow describe the results of the empirical study. The paper concludes with discussing the major conclusions and avenues for future research.

2. CONCEPTUAL CONSIDERATIONS

Consistent with the activity-based approach, we postulate that observed transportation patterns are the result of a complex decision-making process by which individuals try to achieve particular goals in the pursuit of their activities within the spatial-temporal and institutional constraints set by the environment. This section describes the concepts and assumptions underlying the Albatross model regarding decision making and choice behavior.

2.1. Decision making
The organization of activities and related travel takes place in the context of an ever-changing physical environment, an uncertain transportation environment and multi-day variations in planned and unplanned activities that need to be completed. It is postulated that activity participation, allocation and implementation fundamentally take place at the level of the household. It is at that level that particular activities need to be performed, and it is also the household that is involved in the decision which activities to conduct. The actual generation and execution of activity calendars, programs and schedules covers a multitude of time frames.

First, long-term decisions made at the household level strongly influence the generation and composition of activity calendars. Decisions regarding marital status, number of children, and the like, are irreversible or require years to change, and hence have a strong impact on the number and kinds of activities that need to be performed and the constraints that households face. These variables also influence the discretionary

activities, reflecting an assumed relationship between socio-demographic variables and lifestyle. Other long-term decisions, such as choice of residence, choice of work and workplace, and purchase of transport modes can in principle be changed in the short run, but in general represent the kind of choices that are not changed immediately. Hence, these decisions exert a strong influence on possible activity patterns as the location of the residence and workplace vis-à-vis the transportation system represent the main locations of an activity pattern and are the cornerstones of decisions.

Thus, these long-term decisions will influence household activity participation decisions. It is up to household members to allocate these activities to household members. The actual allocation will reflect task allocation mechanisms within the household, which will depend on gender-specific roles, and time pressures. The task allocation and related allocation of activities involves the set of activities that needs to be completed within a particular time horizon. It results in an individual activity program that is derived from the household activity calendar. We postulate that this process of program generation depends on the nature of the activities (mandatory versus discretionary), the urgency of completing a particular activity on a specific day as a function of the history of the activity scheduling and implementation process, and the desire to meet particular activity and time-related objectives.

Once the individual activity program has been generated, the next step is to schedule these activities, which involves a set of interrelated decisions including the choice of location where to conduct a particular activity, the transport mode involved, the choice of other persons with whom to conduct the activities, the actual scheduling of activities contained in the activity program, and the choice of travel linkages which connect the activities in time and space.

These activity scheduling decisions thus transform an individual's activity program into an activity pattern, which is an ordered sequence of activities and related travel at particular locations, with particular start times and duration, with particular transport modes and perhaps coordinated with the activity patterns of other individuals. In this context, travel decisions represent a sub-decision. Transport mode decisions dictate the action space within which individuals can choose locations to conduct their activities. The organization of trips into chains allows individuals to conduct more activities within a specific time frame.

The actual process of scheduling activities is conceptualized as a process in which an individual attempts to realize particular goals, given a variety of constraints that limit the number of feasible activity patterns. Several types of constraints can be identified:

(1) *situational constraints* impose that a person, transport mode and other schedule resources cannot be at different locations at the same time.

(2) *institutional constraints*, such as opening hours, influence the earliest and latest possible times to implement a particular activity.

(3) *household constraints*, such as bringing children to school, dictate when particular activities need to be performed and others cannot be performed.

(4) *spatial constraints* also have an impact in the sense that either particular

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activities cannot be performed at particular locations, or individuals have incomplete or incorrect information about the opportunities that particular locations may offer.

(5) *time constraints* limit the number of feasible activity patterns in the sense that activities do require some minimum duration and both the total amount of time and the amount of time for discretionary activities is limited.

(6) *spatial-temporal constraints* are critical in the sense that the specific interaction between an individual's activity program, the individual's cognitive space, the institutional context and the transportation environment may imply that an individual cannot be at a particular location at the right time to conduct a particular activity.

2.2. Choice behavior

Having identified these constraints, the next question then is how individuals choose between feasible activity patterns. Unlike other models, which relied on utility-maximizing theory, we assume that choice behavior is based on rules that are formed and continuously adapted through learning while the individual is interacting with the environment (reinforcement learning) or communicating with others (social learning).

Assume that an individual has just moved to a new city, which he does not know. To conduct his activities the individual will need to become involved in active search. Consider the choice of a location for shopping as an example. He may try locations at random, ask colleagues, consult newspapers or use some other strategy, but the result will be that he will visit a particular location for shopping. The experience with this location may not satisfy his expectations, in which case the individual will continue his active search behavior. He may, however, also be pleased with the experience. Having tried several locations, he will be able to compare the utilities associated with the different locations, and decide which location is the best under which conditions (travel mode, specific activity, time of the day, day of the week, etc.). He may even induce from specific experiences the attributes of locations that co-vary with particular outcomes. In this way, associations between conditions and actions are formed.

The complexity of condition-action associations may vary from individual to individual depending on the learning history. In particular, the choice between exploration and exploitation is a well-known dilemma in reinforcement learning theory (see Sutton and Barto 1998). Risk takers may prolong exploration and accept the risk of negative outcomes to find choice alternatives that are more rewarding than the current best choice. Risk avoiders, on ther other hand, may stop searching already in an early stage and accept the currently best choice while many alternatives have not been tried. As individuals may display different tendencies, we expect to find a wide variety of choice heuristics in terms of the extent to which context variables and choice alternative attributes are taken into account within a given population.

Given some tendency to explore, refinement of condition-action associations will reflect the complexity of condition-reward contingencies in the environment. In dense urban areas and strong insitutionalized environments, for example, we expect more

differentiated behavior. Household setting, lifestyle and other factors determining complexity and time pressure on activities also have an impact. Moreover, associations tend to change over time. Existing associations may be weakened and new ones formed if the environment, preferences or life cycle of the individual changes.

In sum, the learning theory on which Albatross is based implies that rules governing choice behavior are heuristic, context-dependent and adaptive in nature. The implications of this theory for modeling choice behavior is considered in Section 4.

3. THE SCHEDULING MODEL

The proposed model consists of three components: (1) a model of the sequential decision making process; (2) models to compute dynamic constraints on choice options and (3) a set of decision trees representing choice behavior of individuals related to each step in the process model. The first two components are a-priori defined, whereas the third component is derived from observed choice behavior of individuals. The method used to represent and derive decision rules will be explained in the next section. This section describes the first two components. First, we outline the model assumptions.

3.1. Assumptions
The model considers a particular household and a particular day as given and generates a schedule for maximally two household heads. The presence of children is taken into account as an independent variable in the model, but activities of children are not explicitly represented. A distinction is made between an activity and an activity episode. An activity refers to the collection of all activities of a certain category (e.g., shopping) whereas an activity episode is defined as the time period of uninterrupted participation in a same activity by the same person and at the same location (Bhat and Koppelman 2000). The system generates a schedule in terms of an ordered list S_r for each member r of the household simulated. Each element of S_r represents an activity episode described in terms of relevant profile dimensions including activity type, travel party, duration, start time, location, and if traveling to the location is involved, transport mode and travel time.

Mandatory activities, such as work or school, are typically fixed in a short time horizon of a day. As the model focuses on daily scheduling, the selection, location, duration and start time of such fixed activities are considered given. The model conveniently assumes that fixity of activities is given by a classification of activity type, even though there is some evidence that fixity of activities may vary within activity categories (Doherty 2001). Following Kitamura and Fujii (1998), we will use the term schedule *skeleton* to refer to the fixed and given part of the schedule. Similarly, the model assumes that the distinction between in-home and out-of-home location of activities is given by the activity clasification, implying for example that eating out-of-home is a distinct category from eating in home.

Given the activity skeleton, scheduling involves decisions to add optional activities, hereafter referred to as *flexible* activities, and determining the schedule position and profile of activities. The proposed scheduling process model intends to simulate how individuals frame choices and arrange them into a sequence when they schedule their

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activities. Evidence suggests that individuals tend to schedule their activities in a priority based, rather than time sequential way (Doherty 2000, Ettema *et al*. ..). The schedule position and timing attributes of higher-priority activities tend to be scheduled first and, if there is space left in the schedule, lower-priority activities are considered next. Although the same studies also provide some evidence that the style of scheduling varies considerably between individuals, Albatross presently assumes a pre-defined sequence of choice facets based on an assumed priority ranking of activities by type and an assumed priority ranking of activity attributes.

3.2. The process model
Figure 1 schematically shows the process model. The model first decides on the transport mode for the work activity. Mode choice for work is considered the highest-priority decision because this choice determines which person can use the car for a substantial part of the day in cases where there is only one car and more than one driving license available in the household.

Step 2 determines the activity composition of the schedule. For each flexible activity category, a decision whether or not to add an episode of that activity to *S* is made. If an activity is added, travel party and duration of the activity are determined before a next activity category is considered. This reflects the assumption that travel party and duration further define the nature of the activity. For example, individuals may consider a leisure activity of long duration together with others as qualitatively distinct from a leisure activity of short duration performed alone. Duration is determined in a qualitative way as a choice between a long, average and short episode. Each duration class is defined by a time range depending on the activity category under concern. Temporal constraints define the feasibility of both selection and duration decisions in this step.

Step 3 determines the time of day for each flexible activity in order of priority. This is modelled as choosing a time period for the activity based on a given subdvision of the day (e.g., early morning, late morning, around noon, etc.). The time period constrains the start time of the activity. Based on this the model determines a preliminary position in the schedule. In some cases, the choice of time-of-day uniquely determines a position. In other cases, there remains a choice between several feasible positions. In these cases, the model chooses the position with the shortest time window, to maximize freedom of choice for next activities.

Step 4 determines trip links between activities by choosing for each activity in order of priority whether it is conducted on a Before stop (directly before another out-of-home activity in the schedule) an After stop (directly after another out-of-home activity), an In-between stop or on a single stop trip. The choices made in this stage have several implications for the schedule. First, the activity is repositioned if needed to realize the chosen trip link. After this step, the position of the activity is considered definite. Each activity with a definite schedule position can serve as a basis for a trip link for activities considered next. Thus, trip links can be established between flexible activities as well. Second, in-home activities are inserted where needed to make the schedule consistent with chosen trip links.

In this stage, the tours included in the schedule are identifyable as sequences of one or more out-of-home activities that start at home and end at home. *Step 5* involves a choice of a transport mode for each tour assuming that there are no mode changes between trips

within tours. Tours including a work activity take on the mode that was chosen for the work activity in the first step.

Finally, *step 6* determines the location of each flexible activity in order of priority. For each location choice, the system defines a dynamic location choice-set, dependent on the time-window for the activity, available facilities, opening times of facilities, travel times and minimum activity duration. The decision is modeled as a choice among possible heuristics for selecting a location. The heuristics define alternative ways of trading-off travel distance against attractiveness. Because individuals may choose also inferior locations in terms of these characteristics (e.g., travel longer for a less attractive location), the option 'other' is included. If 'other' is chosen, the model chooses a travel-time band in which the destination location falls. If there is more than one location in the choice set within the chosen band, the location is determined randomly.

The model constructs a schedule for each (adult) person in the household simultaneously by alternating decisions between persons. For each person and each step, the model takes the schedule of the partner as far as developed at the end of the previous step as input to take possible interactions of scheduling choices between persons into account. Finally, we note that start time and duration of flexible activities are not exactly determined by the model. With regard to start time, the time-of-day and trip links with previous and next activity are known. Hence, unless the activity is linked with a fixed activity (with presumably known start and end time), there still remains a choice of start time within some range. The same holds for duration.

In each step, dynamic constraints determine which choice alternatives are feasible given the current state of the schedule. In many cases there will be a choice left and the decision tree linked to that step is consulted to generate a choice. Socio-economic attributes of the person and household are input to take possible interindividual differences in choice heuristics into account. History dependence of decisions is taken into account by including outcomes of previous decisions as input to each current decision. In this way, for example, the probability of adding an activity will be strongly reduced when an activity of that category already has been added in a previous step.

3.4. The inference system

This model component represents dynamic constraints of the types described in Section 2. For each decision, the model evaluates dynamic constraints to determine the feasibility of choice alternatives. The implementation of situational, household and temporal constraints is straightforward. This section focuses on space-time constraints and choice heuristics determining location choices (step 6).

A location *l* is considered feasible if the following two conditions are met:

$$\exists g \in G_l, g \in G\{ a(\tau) \} \tag{1}$$

$$T_{l_g}^{f\,max}(\tau) - T_{l_g}^{s\,min}(\tau) \geq v^{min}(\tau) \tag{2}$$

where, τ is an index of activities in a given schedule *S*, G_l is the set of known facility types at location *l*, $G\{ a(\tau) \}$ is the set of facilities compatible with activities of type $a(\tau)$, $v^{min}(\tau)$ is the minimum duration and $T_{l_g}^{s\,min}$ and $T_{l_g}^{f\,max}$ define the time window for

the activity dependent on the current schedule and opening hours of facilities. The latter terms are formally defined as:

$$T_{l_g}^{f\max}(\tau) = \max\{_d t_{l_g}^{\min}, T^{f\min}(\tau-1) + t_l^t(\tau)\} \tag{3}$$

$$T_{l_g}^{s\min}(\tau) = \min\{_d t_{l_g}^{\max}, T^{s\max}(\tau+1) - t_l^t(\tau+1)\} \tag{4}$$

where, $_d t_{l_g}^{\min}$ and $_d t_{l_g}^{\max}$ are the known opening and closing times of facilities of type g at location l on day d, $T^{f\min}$ is the earliest end time and $T^{s\max}$ the latest start time of the previous and next activity respectively and t_l^t is travel time to the activity location using the mode chosen in a previous step. Earliest start times and latest end times of activities are calculated by shifting previous activities as far as possible to the right on the time scale and next activities as far as possible to the left within temporal constraints.

Having defined the location choice set, the proposed set of heuristics then define alternative ways of trading-off required travel time against attractiveness of locations. Before formulating the heuristics, two concepts must be clarified. First, the *order* of locations refers to an ordinal judgement of the availability of facilities at a location. The classification may relate to a hierarchy of locations. For example, in the Dutch context, shopping centers can be classified into three or four orders that range from neighborhood centers to city centers. The assumption here is that individuals tend to evaluate alternative locations in such qualitative terms. Second, a location is considered *inferior* if it is dominated by at least one alternative in terms of both travel time (shorter) and order (higher). For example, l_1 is dominated by l_2, if l_1 incurs more travel time and is of lower or equal order compared to l_2.

Let L be the choice set for the given activity defined by equations (1) – (4), $L^+ \subseteq L$ be the subset of non-inferior locations, t_l^t be the travel time to location l, $r_1 < r_2 < r_3 < .. < r_m$ be pre-defined critical travel times of increasing lengths, $R_r \subseteq L$ be the subset of locations reachable within travel time r. Then, the heuristics can be written as:

h_1:   choose location l if $l \in L^+ \wedge t_l^t = \min_{l' \in L}(t_{l'}^t)$

h_2:   choose location l if $l \in L^+ \wedge o_l = \max_{l' \in L}(o_{l'})$

$h_{3.1}$:   choose location l if $l \in L^+ \wedge l \in R_1 \wedge o_l = \max_{l' \in R_1}(o_{l'})$

$h_{3.2}$:   choose location l if $l \in L^+ \wedge l \in R_2 \wedge o_l = \max_{l' \in R_2}(o_{l'})$

...

$h_{3.m}$:   choose location l if $l \in L^+ \wedge l \in R_m \wedge o_l = \max_{l' \in R_m}(o_{l'})$

h_4 use some other heuristic

The first two heuristics represent extreme cases where individuals minimize travel time irrespective the order of locations (h_1) or maximize order irrespective required travel time (h_2). The heuristics $h_{3.1}$- $h_{3.m}$ represent the choice for some optimum taking both travel time and order into account. They define a maximum travel time and select the location that maximizes the order within reach. As a set, the heuristics $h_{3.1}$- $h_{3.m}$ represent an

increasing willingness to travel further in order to reach locations of higher order. In all these heuristics non-inferiority is included as a condition to make sure that a possible tie on one criterion (e.g., same travel time) is resolved by a non-inferior choice on the other criterion (e.g., higher order). However, individuals do not necessarily select only non-inferior locations. The last heuristic covers the case where individuals choose an inferior location possibly based on characteristics not represented in the model.

It is easy to verify that heuristics h_1-$h_{3.m}$ may overlap in the sense that, dependent on choice-set L, multiple heuristics may identify the same location. For example, the nearest location and the highest order location may be the same location. To resolve such ambiguities, the proposed model ranks heuristics based on a criterion of explanatory simplicity. The 'nearest location' rule (h_1) is considered simpler than the maximum-travel-time rule, which in turn is considered simpler than the 'highest-order' rule (h_2). If a conflict arises, the simplest heuristic is taken as the rule underlying the observed choice.

Furthermore, it is easy to see that the set of heuristics is not exhaustive in the sense that it not necessarily covers all locations in the choice-set. Let L^h represent the subset of locations that are defined by at least one of the heuristics. Then, the complementary subset L^o consists of locations that are inferior or lie beyond a maximum travel-time. Clearly, individuals may also select inferior locations, for example, a location that performs highly on some other unknown attribute, or use different travel time upper limits. To cover such cases, the proposed model considers a complementary set of heuristics that operates on L^o and considers travel time only. The i-th heuristic of this set considers the subset of locations of L^o that ly in the i-th travel time band and selects from this subset a random location.

Both sets of heuristics assume that individuals evaluate distances to locations in the context of a tour that may consist of multiple activities. Alternatively, individuals may (conditionally) use home-based travel time as a criterion for location selection even if the preceding location or the next location differs from the home location. Therefore, the above set of heuristics (h_1-h_4) can be complemented with an equivalent set based on home-based travel times. We assume that home-based rules are simpler than the tour-based equivalents and, therefore, have higher priority.

4. DECISION TREE INDUCTION

The oval boxes in Figure 1 indicate the places where a decision tree delivers input. This section outlines an approach to derive the decision trees from data and develops a rule for deriving decisions from induced trees. First, we discuss some relevant properties of this rule-based formalism.

4.1. The rule-based formalism
As we argued in Section 2, choice behavior that emerges from learning is driven by individual dependent condition-action rules. In general format, a condition-action rule can be described as:

$$\text{if } C_1 \in CS_{1k} \wedge C_2 \in CS_{2k} \wedge \ .... \wedge C_m \in CS_{mk} \text{ then choose alternative } A_k \tag{5}$$

where C_i represents condition variables, CS_{ik} the condition state of the i-th variable in the k-th rule and A_k the choice generated by the k-th rule. In this notation, a condition state is represented as a subset of the domain of the condition variable. If the condition variable is of a nominal measurement scale, then it may specify any subset of the domain. In the case of an ordinal or metric variable, on the other hand, the condition state specifies a certain subrange of the variable's domain.

To make sure that a rule set is able to respond to every situation, it must meet requirements of completeness and consistency. A model is considered complete if at least one rule responds and consistent if no more than one rule responds to every possible combination of values of condition variables C_i. These properties are guaranteed by the way the learning mechanism operates in our model. Consider an initial situation where the individual has no a-priori knowledge of the domain. Decision-making would be purely random and handled by a single 'rule':

$$\text{if } C_1 \in CD_1 \wedge C_2 \in CD_2 \wedge \ ....\ \wedge C_m \in CD_m \text{ then choose random} \qquad (6)$$

where CD_i represents the domain of condition variable C_i. Since every 'condition state' in this rule equals the entire domain, each variable in effect is irrelevant. Therefore, every possible state in terms of C_i will trigger the rule implying that the model meets the requirements of completeness and consistency. Now assume that through interaction with the environment the individual has learned to discriminate between states on some condition variable. This can be represented by splitting the domain of that variable into two states so that the initial rule is replaced by two new rules:

$$\text{if } C_1 \in CD_1 \wedge C_2 \in CD_2 \wedge \ .....\wedge C_j \in CS_{j1} \wedge .... \ \wedge C_m \in CD_m \text{ then choose A1} \quad (7)$$
$$\text{if } C_1 \in CD_1 \wedge C_2 \in CD_2 \wedge \ .....\wedge C_j \in CS_{j2} \wedge .... \ \wedge C_m \in CD_m \text{ then choose A2} \quad (8)$$

Because the new condition states were achieved by splitting a domain, $CS_{j1} \cup CS_{j2} = CD_j$ and $CS_{j1} \cap CS_{j2} = \varnothing$ and, hence, the new model still meets properties of completeness and consistency[1]. This process of splitting could be repeated endlessly resulting in increasingly complex models while maintaining the required properties.

Besides properties of completeness and consistency, this simple case illustrates that the formalism is consistent with learning theory. Split operations that determine the selection of context and choice attributes an individual evaluates for making a choice may differ from case to case. If search behavior is extensive, condition states are split up to the extent required by the complexity of condition-reward contingencies in the environment. On the other hand, tendencies of limited exploration result in simpler rule sets.

4.2. Inducing decision trees from data
Any set of rules that can be obtained by recursively splitting condition states starting with an initial rule of format (6) meets the formal definition of a decision tree as formulated by

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[1] Our definitions of completeness and consistency do not have any implications for the action section. Although it would not make sense in this example, the two rules could still specify the same action.

Safavian and Landgrebe (1991) and vice versa. Methods based on principles of supervised learning have been developed in statistics and artificial intelligence to empirically estimate decision trees. Supervised learning is learning from examples with known outcomes (in this case, observed behavior). Note that this class of learning is distinct from reinforcement and social learning, where the right answers are unknown and only utilities are fed back to actions of the individual. Hence, the supervised learning technique used here to derive decision trees from data is not seen as a model of a learning process. Rather the technique is used here to find the tree that best describes observed choices. The outcome is considered a model of the current state of knowledge of the individual or group of individuals from which observations were taken.

Examples from which a decision tree is induced describe observations on one or more condition variables (our terminology) and a single response variable. The (minimal) tree that partitions the sample into groups that are maximally homogeneous in terms of the response variable is considered the best hypothesis for the data. Because the number of possible trees increases exponentially with the number of condition variables, work in this area has focused on heuristics to search for the best tree. C4.5 (Quinlan 1993), CART (Breiman *et al*. 1984) and CHAID (Kass 1980) are the most widely used heuristics[2]. All three programs grow a tree from the root by recursively splitting the sample on one condition variable at a time. They differ with respect to the criterion that is used for evaluating possible splits. C4.5 uses an entropy measure and CART the Gini-index to measure purity of a response distribution, whereas CHAID evaluates splits based on a Chi-square measure of significance of differences in response distributions between groups. CHAID further differs in that it uses a stop rule, whereas the other programs first grow a full tree and next prune the tree by removing insignificant branches.

The choice of an induction method for developing Albatross is based on a trade-off between specific strengths of the competing methods. A two-staged process, as employed by C4.5 and CART, is potentially more powerful, because it circumvents to some extent the inherent weakness of looking only one step ahead in selecting splits. By lowering the threshold for splitting in the tree-growing stage splits that pay-off only in combination with other splits are more likely to be identified. On the other hand, CHAID is more sensitive for differences in complete response distributions compared to C4.5 and CART. The entropy measure and Gini-index do take entire response distribution in to account in the growing stage. However, the effects are counterbalanced in the pruning stage, where both methods base pruning decisions primarily on (absence of) differences in modal responses alone.

Arguably, the latter disadvantage of C4.5 and CART outweighs the advantage of a two-staged approach. A model of modal responses ignores residual variance in responses within the partitions created. As will be explained in the next section, Albatross uses a probabilistic rule for assigning responses to cases classified by a tree with the aim to reproduce non-systematic variance in model predictions. In the context of a probabilistic rule the distribution of responses is as important as the modal response. Moreover, in previous comparative studies (Arentze *et al*. 2000 and Wets *et al*. 2000) we found no significant differences in performance between the methods on an activity-data set. It is

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[2] CHAID is usually not considered as a decision tree induction method as it was introduced in statistics as a data segmentation technique. However, because the form of input and output is the same, we consider CHAID to belong to this class of methods (Arentze, Hofman, Van Mourik, Timmermans & Wets 2000).

for that reason that we propose CHAID for developing decision-tree based models such as Albatross.

4.3. Deriving decisions from decision trees
Having derived a decision tree for each choice facet, the next question becomes how to derive decisions from trees for prediction. Consider a response variable that has Q levels and for which CHAID produced a tree with K leaf nodes. In the prediction stage, the tree is used to classify new cases to one of the K leaf nodes based on attributes of the case. A response-assignment rule needs to be specified that defines a response (decision) for each classified case. In many applications, a plurality rule is used. This rule assigns the modal response among training cases (i.e., the sample used for developing the tree) at a leaf node. A deterministic rule like this may yield the best predictions at an individual level, but fails to reproduce residual variance (if any) at leaf nodes in predictions. Given our modeling purpose, we, therefore, use a probabilistic assignment rule instead. According to this rule, the probability of selecting the q-th response for each new case assigned to the k-th node is simply given by:

$$p_{kq} = \frac{f_{kq}}{N_k} \tag{9}$$

where f_{kq} is the number of training cases of category q at leaf node k and N_k is the total number of training cases at that node.

This rule is sensitive to residual variance, but fails to take scheduling constraints into account. Scheduling constraints entail that dependent on individual attributes and the state of the current schedule some choice alternatives for the decision at hand may be infeasible. If such constraints are represented in the decision tree, the probabilistic rule would assign zero probability to infeasible categories and the response distribution should not be biased. However, even though it is likely, it is not guaranteed that the induction method discovers constraint rules in data. Therefore, to cover the general case we need to refine rule (9) as:

$$p_{kq} = \begin{cases} 0 & \textit{if } q \textit{ is infeasible} \\ \dfrac{f_{kq}}{\sum_{q'} f_{kq'}} & \textit{otherwise} \end{cases} \tag{10}$$

where q' is an index of feasible alternatives for the decision at hand. Even though this rule may work well in practice, it may produce slightly biased patterns at an aggregate level that should be noted. That is to say, the rule tends to overpredict responses that are feasible in the majority of cases (at that leaf node), because the probability of these responses is increased by rule (10) in constrained cases and stays the same as (9) in unconstrained cases. Nevertheless, we use rule (10) keeping in mind that improvements are possible.

5. APPLICATION

To develop and test the Albatross model, an activity diary survey was conducted in two municipalities in the Rotterdam region in the Netherlands in 1997. This section discusses the format of the diary data and results of decision tree induction.

5.1. Data

The survey invited households to fill out an activity diary for two consecutive days. Days were designated to households such that the sample was balanced across the days of the week. The activity diary asked respondents, for each successive activity, to provide information about the nature of the activity, start and end time, the location where the activity took place, the transport mode (chain) and the travel time per mode, if relevant, accompanying individuals (alone, other member of household, other), and whether the activity was planned. Open time intervals were used to report the start and end times of activities. A pre-coded scheme including 48 categories was used for activity reporting. Response rates among households that had indicated to be willing to participate ranged between 64 and 82% dependent on mode of administration. This resulted in a total of 2198 household-days that were used for the analysis. The diaries were cleaned using the special-purpose program Sylvia (Arentze *et al.* 1999).

Data of the physical environment were obtained through national databases and fieldwork. The data were aggregated to zip-code zones and included mode-specific shortest-route travel times and distances between zones, size of facilities by sector and opening hours of facilities by sector and day of the week. The size of facilities was measured as total amount of floor space and number of employees per sector. Opening hours data were collected through local inspection of centers and a telephonic survey among outlets, chains and organizations. They were aggregated per zone by calculating the earliest possible opening time and latest possible closing time across outlets. The types of facilities considered included daily shopping, non-daily shopping, service (bank, post office, travel agency, etc.) and leisure facilities (cafe, restaurants, theatre, etc.).

The 48 activity categories used in the diary were classified into 11 broader categories. Table 1 shows the classification used and subdivision into fixed and flexible activities. All flexible out-of-home activities could be related to facilities in the physical data set, except social activities. With respect to social activities, the model assumed that all zones and times are feasible and equally attractive for conducting the activity.

5.2. Results of decision tree induction

The activity diary data was used to derive a decision tree for each decision step in the process model (see Section 3) conveniently assuming that reported activities reflected the activity schedules of individuals[3]. 75% of the cases was used for training (developing the decision trees) and the remaining cases were used for validation testing. For each choice

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[3] In reality, not necessarily all activities that people conduct are planned. Furthermore, during execution the schedule can be adjusted in response to unforeseen events.

facet, the observed choice and attributes of the schedule as far as known in that stage of the assumed decision process were extracted from the diary data.

In general, the attributes considered as potentially relevant condition variables relate to:

1. Person, household and space-time setting
2. Activity program/sequence at schedule level (including partner, if any)
3. Activity program/sequence at tour level
4. Activity profile and space-time setting at activity level
5. Feasibility of choice alternatives at choice-facet level

Socio-economic and space-time setting attributes at person and household level allow CHAID to identify groups of individuals with similar choice behavior. Thus, deriving decision rules and segmenting the population in homogeneous groups in terms of these decision rules is accomplished simultaneously. Available information at schedule, tour, and activity level is initially limited to the schedule skeleton and increases as scheduling proceeds. Because outcomes of previous decisions are included as conditional variables for each next decision step, interactions between choices can be represented explicitly in decision trees. Finally, the last category – feasibility of choice alternatives – is important, because it allows the system to differentiate between choice behavior under constrained and unconstrained conditions.

CHAID allows users to define the threshold for splitting in terms of a significance level for the Chi-square measure and a minimum number of cases at leaf nodes. Alpha was set to 5 % and the minimum number of cases to 20. Because CHAID can handle categorical condition variables only, continuous attributes such as travel times, durations and start times, were discretisized using an equal-frequency method. This method divides a scale into *n* parts in such a way that each part represents approximately the same number of cases.

Table 2 shows input and output characteristics of CHAID per decision tree. The number of leaf nodes gives an indication of the complexity of the resulting tree and the last three columns shows hit ratios as a measure of predictive accuracy. The hit ratio represents the expected number of correctly predicted cases when a probabilistic response-assignment rule of type (9) is used. It is calculated as $\sum_{kq} \dfrac{\left(f_{kq}\right)^2}{N_q}$ where f_{kq} is the frequency of the q-th response at the k-th leaf node and N_k is the frequency of the q-th response in the entire sample.

As it turns out, performance varies considerably across choice facets. Duration, with-whom, location(2) and time-of-day choices are relatively difficult to predict. Partly, this reflects differences in number of choice alternatives. The base probability of correctly predicting choices increases with decreasing number of alternatives. Comparison with expected hit ratios of a null model gives an indication of relative performance. The null model uses the probability distribution at the aggregate level to predict a choice in each case and, hence, simulates a tree with a single leaf node. Relative performance is relatively poor for activity-selection and duration facets and relatively good for location and time-of-day choices. Finally, comparing expected hit ratios between training and test

set gives an indication of generalizability of the model to unseen cases. Since decline in performance is generally small, we conclude that overfitting is not a problem here.

Each decision tree provides valuable information for interpreting choice behavior. To illustrate the use of trees for interpretation, Table 3 shows a branch of the time-of-day tree as an example. The first split in this tree concerns activity type and the branch depicted relates to non-daily shopping activities. The (sub)tree is represented in table format. The upper section of the table shows condition variables and condition states and the bottom section displays the levels of the response variable and response probability distributions of training cases. Note that each column corresponds with a leaf node. The last row shows number of training cases per leaf node.

As can be concluded from the table, time-of-day choices for non-daily shopping are conditioned almost exclusively by patterns of available time in the current schedule. Tmax variables represent for each of four episodes of the day whether and to what extent there is time to conduct the shopping activity (with duration given by a previous decision). As an overall rule, the model tends to select the earliest feasible episode of the day. However, in cases where this episode starts before 12 PM, time-of-day choices become more dispersed. Under less constrained choice situations the preferred time of day stretches from 10 am to 4 PM. The presence of an out-of-home daily shopping activity tends to delay non-daily shopping, whereas the presence of an out-of-home leisure activity tends to lead to earlier start times. In sum, the patterns suggest specific preferences for time-of-day and sequencing of activities and point at a strong influence of temporal constraints. Socio-demographic and space-time setting attributes do not provide additional explanation of choice behavior in this case.

6. PERFORMANCE OF THE ALBATROSS MODEL

The hit ratios shown in Table 2 give an indication of prediction accuracy of each decision tree whereby earlier decisions are given as observed. Choices between choice facets are, however, interrelated in the sense that earlier decisions affect conditions for later decisions. Moreover, decisions derived from trees are part of a scheduling process model that translates decisions to appropriate operations on the schedule. The eventual goodness-of-fit of the model can be assessed only by a comparison at the level of complete activity patterns. Being a travel demand model, the eventual output of Albatross consists of trip matrices. This section evaluates goodness-of-fit at this level. Before discussing the results, we consider some descriptive statistics of the data.

Table 4 shows the means and standard deviations of number of activities of predicted and observed patterns. Because Albatross does not differentiate between in-home activities, consecutive in-home activities in observed patterns were merged to make the sets comparable. After this pre-processing, the mean length of patterns varies between 5.2 and 5.4 activities dependent on the data set. Recall that Albatross considers fixed activities as given. The mean number of flexible out-of-home activities varies between 1.3 and 1.4. The means as well as standard deviations are fairly accurately predicted, be it that the number of activities is slightly overpredicted in the test set.

The study area counts 19 zones. The outside area is considered an additional single zone in the trip matrix. Different matrices were generated varying a third dimension on which interactions were broken down. The third dimensions considered include:

1. No third dimension
2. Transport mode (slow mode, car driver, car passenger and public transport)
3. Day of the week (weekday, Saturday, Sunday)
4. Time of day (before 10 AM, 10 – 12 AM, 12 – 2 PM, 2 – 4 PM, 4 – 6 PM, after 6 PM)
5. Activity (9 categories)
6. Activity (only flexible activities: 5 categories)

Note that the number of cells and, hence, the degree of disaggregation differs between the matrices. For example, the trip matrix by mode has $4 \times 20 \times 20 = 1600$ cells and the trip matrix by activity has $9 \times 20 \times 20 = 3600$ cells. The fifth and last matrix is based on trips with a flexible activity at the destination location only. This matrix is particularly relevant for assessing the performance of the model, because it leaves out trips with locations and activities given by the skeleton.

The correlation coefficient was used as a measure of degree of correspondence between trip matrices. As Table 5 shows, correlations for the test set vary between .706 - .954 dependent on the third dimension. The variation across matrices can be largely explained by the variation in number of cells. As could be expected, goodness-of-fit decreases with increasing number of cells (i.e., the level of disaggregation of interactions). Furthermore, as expected the matrix related to flexible activities shows an extra decline in fit. Overall, however, the results indicate that performance is very satisfactory keeping in mind that patterns are only partly predicted by the model. The difference in performance between training and test set can be expressed as a ratio between test-set and training-set scores. The ratios range between 85-99%. We conclude, therefore, that the extent to which overfitting has occurred is acceptable.

7. CONCLUSIONS AND DISCUSSION

This paper described the conceptual development, operationalisation and validation testing of Albatross. The system simulates individual's decisions related to every facet of activity schedules generally considered relevant for activity-travel analysis. The facets include activity type, duration, travel party, start time, trip type, location and transport mode. The system is designed as a rule-based model in which situational, household, institutional and space-time constraints as well as choice heuristics of individuals are explicitly represented in the system.

Central to the proposed approach is the use of the decision tree for representing choice heuristics of individuals and deriving these heuristics from activity travel data. As it appeared, the decision tree achieved a considerable, but varying improvement of predictive accuracy compared to a null model and the results could be replicated on a validation set. Correlations between observed and predicted trip matrices indicated that the model is able to explain a large proportion of observed variance across intensities of trip flows disaggregated on various dimensions relevant for travel analysis.

We conclude therefore that the approach is useful for developing computational process models for forecasting travel demands. We motivated the choice for a rule-based approach based on a theory of how people learn in complex environments. Potentially,

decision trees are better able to represent the heuristic and context dependent nature of choice behavior compared to current utility-maximizing models. Although decision tree induction requires relatively large data sets, this research shows that a sample size of the order of magnitude of 2000 household-days suffices to develop a stable model and test the validity of the model. Nevertheless several issues remain for future research.

First, the generalizability of the present model was tested on a holdout sample. Because the holdout sample originated from the same study area and the same survey instrument, this is more a test of internal validity than external validity. The question remains how well the model would perform when applied in another study area. Transferability of a model to another context than in which it was developed has received some attention in the area of discrete choice modeling (Koppelman and Wilmot, 1982). Such transferability studies need to be replicated in this new area of rule-based models. The ability to predict reactions of individuals to transportation or spatial policy scenarios is a specific form of transferability that is of particular interest. On all of these criteria of internal and external validity it is worth while to compare the rule-based approach with equivalent utility-based models. Such comparative studies would provide an indirect test of validity of the specific assumptions underlying the rule-based model.

Besides testing the current model, several extensions of the model are worth considering. First, decision tree induction techniques use principles of supervised learning and, therefore, are not suitable for modeling individuals time paths of learning and adaptation. To model time paths as well, models of reinforcement and social learning need to be developed and incorporated in the system. Potentially, the resulting dynamic model would be able to predict and analyze long-term impacts of policy measures or trends in society.

Second, we mention possible extensions at the level of the process model. Although the current process model is already quite comprehensive compared to existing activity-based models, several extensions could increase sensitiveness of the model for relevant travel demand measures. These cover areas of 1) joint decision making and interactions between persons within households, 2) long term decision making related to choice facets of the schedule skeleton, 3) re-scheduling behavior during schedule execution, 4) individual and context varying styles of scheduling and 5) in-home versus out-of-home activity substitution choice behavior.

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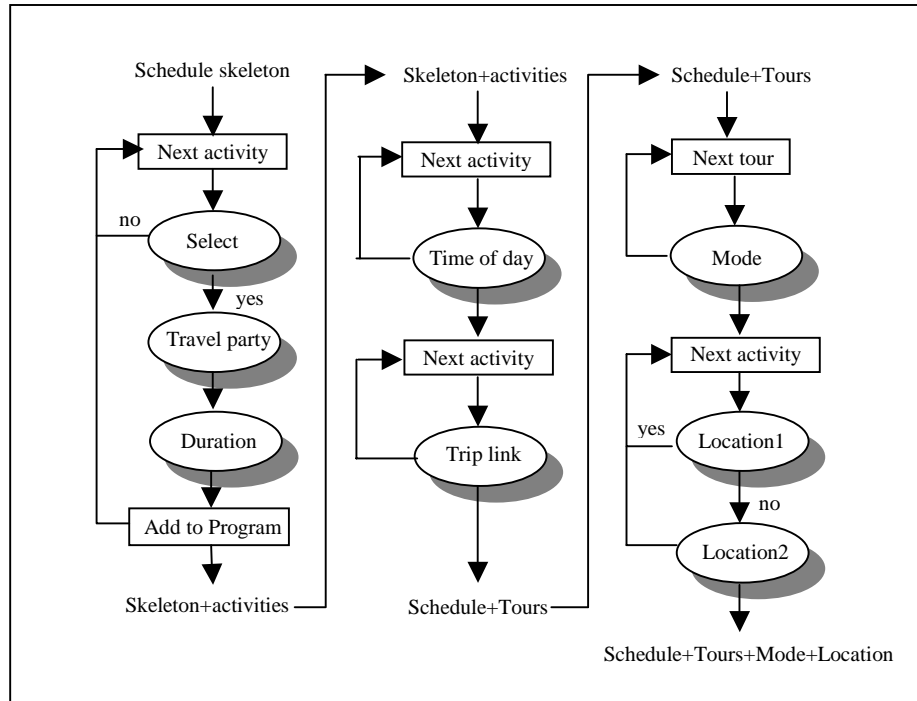
Figure 2. The scheduling process model (step 2-6)

Table 1. Classification of activities used in the Albatross model.

Fixed activities	Flexible activities
work / school	daily shopping
bring or get persons or goods	service related activities (post office, bank etc.)
medical visits	non-daily shopping
personal business (a rest category)	social activities (visiting friends, relatives etc.)
sleep and eat	leisure activities (sports, concert, library, restaurant etc.)
	home-based activities (other than sleep and eat)

Table 2. Results of inducing decision trees from diary data by choice facet

Decision tree	N alts	N cases	N Attr	N leafs	hit r(0)	hit r (t)	hit r (v)
1. Mode for work	4	858	32	23	.525	.648	.667
2. Activity selection	2	14190	40	116	.669	.724	.716
3. Activity, with-whom	3	2970	39	57	.335	.509	.484
4. Activity, duration	3	2970	41	61	.334	.413	.388
5. Activity, time-of-day	6	2970	62	86	.172	.398	.354
6. Trip link	4	2651	52	30	.533	.833	.809
7. Mode for other	4	2602	35	65	.388	.528	.495
8. Activity, location 1	7	2112	28	62	.375	.575	.589
9. Activity, location 2	6	1027	28	34	.326	.354	.326

N alts	Number of choice alternatives	hit r (0)	Expected ratio of correctly predicted cases (null model)
N cases	Number of training cases	hit r (t)	Expected ratio of correctly predicted cases (training set)
N attr	Number of attributes	hit r (v)	Expected ratio of correctly predicted cases (test set)
N leafs	Number of leaf nodes		

Table 3. Example of a decision tree: time-of-day of non-daily shopping activities.

yDshop	-	-	-	-	-	0	1	-	-	0	0	1
yLeis	-	-	-	-	-	-	-	-	-	0	1	-
Tmax1	0	0	0	0	0	0	0	1	2-3	2-3	2-3	2-3
Tmax2	0	0	0	0	1-2	3	3	-	-	-	-	-
Tmax3	0	0	1-2	3	-	-	-	-	0	1-3	1-3	1-3
Tmax4	0	1-3	-	-	-	-	-	-	-	-	-	-
< 10 am	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.32	0.25	0.16	0.08	0.05
10-12 am	0.00	0.00	0.00	0.00	0.41	0.47	0.23	0.37	0.29	0.15	0.42	0.13
12-2 pm	0.00	0.00	0.90	0.40	0.35	0.13	0.23	0.21	0.00	0.34	0.14	0.42
2-4 pm	0.00	0.81	0.11	0.48	0.24	0.22	0.50	0.05	0.21	0.27	0.33	0.30
4-6 pm	0.50	0.12	0.00	0.04	0.00	0.18	0.05	0.05	0.14	0.08	0.03	0.05
> 6 pm	0.50	0.08	0.00	0.08	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.06
N	30	26	19	25	37	60	22	19	28	74	36	64

yDshop   There is a daily shopping activity in the schedule (0 = no, 1 = yes)
yLeis   There is a out-of-home leisure activity in the schedule (0 = no, 1 = yes)
Tmax1-4   Available time in the widest open time slot within episode 1-4 of the day (0 = insufficient, 1 = sufficient and 2 = more than sufficient)

Table 4. Mean number of elements in patterns (standard deviation between brackets).

	Training data		Test data	
	Observed	Predicted	Observed	Predicted
N activities (total)	5.328 (2.653)	5.357 (2.817)	5.230 (2.540)	5.441 (2.762)
N activities (flexible)	1.343 (1.213)	1.293 (1.247)	1.287 (1.174)	1.352 (1.269)

Table 5. Contingency and correlation measures between predicted and observed OD matrices.

	Training data	Test data
None	0.966	0.954
Mode	0.933	0.887
Day	0.969	0.962
Time of day	0.970	0.953
Activity	0.896	0.845
Activity (flex)	0.832	0.706