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CHOICE MODEL SPECIFICATION, SUBSTITUTION AND SPATIAL STRUCTURE EFFECTS
A Simulation Experiment

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Several choice models are compared on their ability to reproduce two types of simulated data sets. The sets belonging to the first type were generated by using a probit model which is able to account for substitution effects while the data sets of the second type were generated by using a probit model which is able to account for spatial structure effects. The main conclusion of the experiment is that simple models like the multinomial logit model, although they perform less than the models used to generate the data, are sufficiently robust to reproduce the simulated data.

1. Introduction

Recently, discrete choice models have found increasing application in urban and regional economics [for a review see e.g., Fischer and Nijkamp (1984) and Wrigley (1985)]. Notwithstanding their popularity, especially the multinomial logit (MNL) model has not escaped criticism. First, the MNL model has been criticized in that the model predicts choice probabilities to be independent of the size and the composition of the choice set and consequently does not incorporate substitution effects. When substitution effects exist, the introduction of a new choice alternative reduces the probability of dissimilar choice alternatives less than when substitution effects are absent. Substitution effects are at their maximum when, after introducing a new choice alternative, the choice probability of one or more of the existing choice alternatives alters while the choice probabilities of the remaining existing choice alternatives are unaffected, which is only possible when the new choice alternative is identical to one or more of the existing choice alternatives.

Second, following similar arguments as Fotheringham (1983a, b, 1984, 1985) has put forward in the context of spatial interaction models, discrete
choice models can be criticized in that these models are not sensitive to spatial structure effects. Such effects exist when spatial choice behaviour depends on the spatial arrangement of the choice alternatives. At least two types of spatial structure effects can be distinguished [Fotheringham (1985)]: competition effects and agglomeration effects. Competition effects exist when two choice alternatives, located relatively close to each other, increase the choice probability of other alternatives. In contrast, agglomeration effects exist when these two choice alternatives decrease the choice probability of other alternatives. Spatial structure effects can be at their maximum only when two choice alternatives are located at the same location. Assume that a new choice alternative will be located at the location of another, equally attractive choice alternative. In this case, competition effects are at their maximum when the sum of the choice probabilities of both alternatives is equal to the choice probability of the existing choice alternative before the new alternative was introduced.

Recently, the authors have extended Kamakura and Srivastava's (1984) substitution model to produce a spatial choice model which is able to account simultaneously for both substitution and spatial structure effects [Borgers and Timmermans (1985a)]. Although this probit model is preferable from a theoretical point of view, the question remains whether this model outperforms existing, mostly less complicated, choice models. Ultimately, this appears to be a problem of empirical analysis, but first, it may be valuable to investigate the ability of existing choice models to reproduce data with known properties, generated by the extended Kamakura and Srivastava model. The latter problem constitutes the purpose of this study.

The paper itself is organized as follows. First, in the next section, the models used in the present experiment are briefly described. This is followed, in section 3, by a description of the simulation method used to generate the data for the experiment. Section 4 then presents the findings of the simulation experiment. The paper is concluded with a summary and discussion.

2. The selected choice models

Especially over the last decade, various choice models have been developed which are able to account for substitution effects and/or spatial structure effects [see Timmermans and Borgers (1985) for an extensive overview]. In this paper, particular attention will be paid to those choice models that are relatively easy to estimate and easy to use for predicting the likely effects of policy measures [for a detailed discussion, see Borgers and Timmermans (1985a)].
2.1. Substitution models

Three classes of substitution models may be distinguished. The first class includes a number of models which impose more general conditions on the variance–covariance matrix of the error terms. In contrast to the multinomial logit model which is characterized by identically and independently double exponential distributed error terms, these models allow dependently and/or not identically distributed error terms. Examples are the negative exponential distribution model proposed by Daganzo (1979), McFadden's (1978) extreme value model, the cross-correlated logit model introduced by Williams (1977), the generalized probit model [see Daganzo (1979)], the perceptual interdependence model proposed by Hausman and Wise (1978) and Kamakura and Srivastava's (1984) probit model. Only these last two models are [by using Clark's (1961) or Langdon's (1984) approximation method] relatively easy to estimate and easy to use for prediction purposes, while under certain conditions these models can also account for maximum substitution effects. Hence, these two models were selected from the first class of substitution models. Both these probit models can be expressed by using the general random utility model

\[ p_i = \Pr \{ U_i > U_j ; \forall j \neq i \}, \quad \text{where} \]

\[ p_i \] is the probability that choice alternative \( i \) will be chosen,
\( U_i \) is the utility of alternative \( i \).

The utility of an alternative is commonly defined as

\[ U_i = V_i + e_i, \quad \text{where} \]

\[ V_i = \sum_k \beta_k X_{ik}, \]

\( X_{ik} \) is the score of alternative \( i \) on attribute \( k \),
\( \beta_k \) is a weight for attribute \( k \),
\( e_i \) is the random utility component of alternative \( i \).

For probit models in general, the random utility components are multivariate normal distributed with zero mean and a particular variance–covariance matrix. In the Hausman and Wise model, the random components are
assumed to consist of two elements:
\[ e_i = \beta_k^* X_{ik} + e_i^* , \]  
where
\[ \beta_k^* \] is a random taste parameter,
\[ e_i^* \] is a random error term.

If the \( \beta_k^* \)'s and \( e_i^* \)'s are uncorrelated, it follows that the elements of the variance–covariance matrix of the perceptual interdependence model are defined as
\[
\text{VAR}_{ij} = \sum_k \text{VAR}(\beta_k^*) X_{ik} X_{jk} \text{VAR}(e_i^*) ,
\]
where
\[ \text{VAR}(\beta_k^*) \] is the variance of the \( \beta_k^* \)-terms,
\[ \text{VAR}(e_i^*) \] is the variance of the \( e_i^* \)-terms.

For estimation purposes it is straightforward to set the \( \text{VAR}(e_i^*) \)-terms to a constant. Only when this constant is equal to zero, the perceptual interdependence model is able to account for maximum substitution effects. The elements of the variance–covariance matrix for the Kamakura and Srivastava model are defined as
\[
\text{VAR}_i = s_i^2 ,
\]
\[
\text{COV}_{ij} = s_i s_j R_{ij} ,
\]
where
\[ \text{COV}_{ij} = \theta \exp (-\alpha r_{ij}) ,
\]
\[ r_{ij} = \left[ \sum_k \beta_k^2 (X_{ik} - X_{jk})^2 \right]^{0.5} ,
\]
\[ s_i \] is the standard deviation of the \( e_i \)-terms,
\[ \theta, \alpha \] are substitution parameters to be estimated, \( 0 \leq \theta \leq 1 \), \( \alpha \geq 0 \),
\[ \beta_k \] represents the weight of attribute \( k \) in the structural utility component.

By assuming homoscedasticity \( (s_i = c, \forall i) \), the model becomes more parsimonious.

The second class of models consists of choice models which account for substitution effects by extending the conventional MNL model formula. Examples are the dogit model [Gaudry and Dagenais (1979)] and models
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proposed by Batsell (1981), Meyer and Eagle (1981, 1982), Huber (1982), Huber and Sewall (1982), Borgers and Timmermans (1984) and Cooper and Nakanishi (1983). The dogit model and the model proposed by Huber and Sewall (1982) will not be discussed in this paper because they are not easy to use to predict the likely effects of policy measures. The model by Huber (1982) will not be considered because of its unrealistic assumptions.

The model proposed by Cooper and Nakanishi (1983) is an ordinary logit model which uses scaled attribute values. The so-called zeta-squared transformation is defined as

$$Z_{ik}^2 = \begin{cases} 1 + Z_{ik}^2 & \text{if } Z_{ik} \geq 0, \\ (1 + Z_{ik}^2)^{-1} & \text{if } Z_{ik} < 0, \end{cases}$$

where

$$Z_{ik} = \frac{X_{ik} - \bar{X}_k}{\sqrt{1/N \sum_j (X_{jk} - \bar{X}_k)^2}}.$$

$\bar{X}_k$ is the mean score for attribute $k$, $N$ is the number of choice alternatives.

However, rather than using zeta-squared scores, one may also use zeta scores or Z scores. In contrast to the Z transformation, which is a linear transformation, the Z and $Z^2$ transformations are non-linear. None of the transformations alters the rank ordering of the original scores. According to some examples of Cooper and Nakanishi (1983), the zeta squared transformation should be the most appropriate transformation when choice behaviour is affected by extreme substitution effects.

The remaining models belonging to the second class of choice models can in general be expressed as

$$p_i = \frac{R_i \exp(V_i)}{\sum_j R_j \exp(V_j)},$$

where $R_i$ is a positive measure of the average degree of dissimilarity between alternative $i$ and all other choice alternatives.

The models basically differ only in terms of the definition of the $R_i$-measure. Batsell (1981) defined this measure as

$$R_i = \exp \left( \frac{1}{N} \sum_k \sum_j \theta_{ik} |X_{ik} - X_{jkl}| \right).$$
and Meyer and Eagle (1981, 1982) as

$$R_i = \left[ \frac{1}{N} \sum_{j \neq i} 0.5 |r_{ij} - 1| \right]^\theta,$$

where \( r_{ij} \) is the observed Pearson product moment correlation between alternatives \( i \) and \( j \) across their attributes,

while Borgers and Timmermans (1984) defined the dissimilarity measure as

$$R_i = \prod_k \left[ \frac{1}{(N-1)} \sum_j |X_{ik} - X_{jk}| \right]^{\theta_k},$$

where \( K \) is the number of attributes.

The Meyer and Eagle (1981, 1982) model contains a parameter \( \theta \) (\( 0 \leq \theta \leq 1 \)) which indicates the strength of the substitution effects. When this parameter equals zero, substitution effects are absent and the model reduces to the conventional MNL model. The Batsell (1981) model and the model proposed by Borgers and Timmermans (1984) contain a substitution parameter \( \theta_k \) (\( 0 \leq \theta_k \leq 1 \), \( \forall k \)) for each attribute. Each parameter \( \theta_k \) indicates the extent to which the corresponding attribute contributes to the substitutability of the choice alternatives. When all parameters \( \theta_k \) are equal to zero, substitution effects are absent and the models reduce to the MNL model.

It should be noted that, in contrast to the selected probit models, the models belonging to the second class of substitution models always yield similar choice probabilities for alternatives with similar deterministic utility components and similar dissimilarity measures.

A third class of substitution models contains models with a hierarchical or sequential decision structure. Examples are the well-known nested logit model [see e.g., McFadden (1978) and Sobel (1981)], the elimination by aspects model [Tversky (1972a, b)], the hierarchical elimination models [Tversky and Sattath (1979)] and the choice by feature model [Strauss (1981)]. These models will not be considered in this paper because they are difficult to use as a planning tool, they are difficult to calibrate or they need an a priori determined decision structure. In some research contexts, such a decision structure may be obtained rather easily, but in studies where many different choice alternatives are available, the derivation of the decision structure appears to be rather arbitrary. In addition, Strauss' choice by feature model is characterized by the assumption that the Luce model (an IIA-model) is appropriate for each attribute separately, which is in the context of this study rather unrealistic.
2.2. Spatial structure models

Borgers and Timmermans (1984, 1985a,b) have proposed two choice models which are able to account for spatial structure effects. Both these models are also able to account for substitution effects. However, to present strictly spatial structure models, the substitution terms in these models are deleted from the models formulae. The first model, the spatial structure logit model [Borgers and Timmermans (1984)], reads as follows:

$$p_i = \left[ \frac{D_i^\phi \exp(V_i)}{\sum_j D_j^\phi \exp(V_j)} \right], \quad \text{where}$$

$$D_i = \frac{1}{(N-1)} \sum_j d_{ij},$$

\(d_{ij}\) is the distance between alternatives \(i\) and \(j\), \(\phi\) is a spatial structure parameter, \(\phi \leq 1\).

Agglomeration effects are indicated by a negative \(\phi\)-value while competition effects are indicated by positive \(\phi\)-values.

The second model [Borgers and Timmermans (1985a, b)] is an analogy of the substitution model proposed by Kamakura and Srivastava (1984). Now, the covariances in the variance–covariance matrix are defined as

$$\text{COV}_{ij} = s_i s_j f(d_{ij}), \quad \text{where}$$

\(f(d_{ij})\) is a function of the distance between alternative \(i\) and alternative \(j\), 
\(-1 \leq f(d_{ij}) \leq 1\).

The function \(f\) in this spatial probit model can be defined in several ways, for example:

$$f(d_{ij}) = \phi \exp(-\gamma d_{ij}) - 0.5,$$

where \(\phi, \gamma\) are parameters, \(-0.5 \leq \phi \leq 0, \gamma \geq 0\).

In this case, locating two choice alternatives closer to each other reduces the choice probability that one of the remaining choice alternatives will be chosen.

3. The simulation experiment

To assess the ability of the models to reproduce data generated by the Kamakura-Srivastava substitution probit model respectively the spatial structure probit model, a simulation was conducted to generate two types of
data sets. Two data sets, the 'substitution sets', were generated by assuming the same choice behaviour as that underlying Kamakura and Srivastava's probit model. Two other data sets, the 'spatial structure sets', were generated by assuming agglomeration effects according to the spatial structure probit model. The first 'substitution set' and the first 'spatial structure set' were generated to estimate the parameters of the choice models. The second 'substitution set' and the second 'spatial structure set' were generated to determine the performance of the calibrated models after introducing a new choice alternative.

The data sets were generated in the context of spatial shopping behaviour. For that purpose, an imaginary part of a city was constructed in a square area of 50 by 50 distance units. The centre of this area was assumed to contain a large shopping centre, while the north-eastern part of the area contains a number of small shopping centres. Further, some medium sized shopping centres were located randomly. In table 1, the characteristics (floorspace and price setting) and locations of the shopping centres are summarized. These attribute scores and locations were determined such that substitution effects and spatial structure effects are able to affect consumers' choice behaviour. However, to approximate real world shopping behaviour as closely as possible, no principles according to some design were used to determine the characteristics and locations of the shopping centres.

The simulation experiment was performed for 100 consumers. For each consumer, his location of residence, the distances between residence and the shopping centres, the number of known shopping centres, his familiarity with the shopping centres and the number of times that each of the known

<table>
<thead>
<tr>
<th>Centre</th>
<th>x-coord</th>
<th>y-coord</th>
<th>Floor space</th>
<th>Price setting</th>
</tr>
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<tr>
<td>1</td>
<td>5</td>
<td>70</td>
<td>5</td>
<td></td>
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<tr>
<td>2</td>
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<td>8</td>
<td>41</td>
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<td>9</td>
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<td>10</td>
<td>46</td>
<td>5</td>
<td>50</td>
<td>8</td>
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<tr>
<td>11</td>
<td>47</td>
<td>48</td>
<td>50</td>
<td>6</td>
</tr>
<tr>
<td>12</td>
<td>49</td>
<td>40</td>
<td>50</td>
<td>8</td>
</tr>
</tbody>
</table>

*A large number indicates a cheap shopping centre.*
shopping centres will be chosen were determined according to a series of rules.

(1) The location of residence was determined by drawing twice a random number between 0 and 50. These two numbers constitute the \( x \) and \( y \) coordinate of the consumer's residence.

(2) Given the consumer's residence, the scores on the third attribute, the distance to the shopping centres, were determined by calculating the Euclidean distance between the consumer's residence and the location of each shopping centre. The attribute scores of the alternatives as perceived by the consumer were determined by adding a disturbance term to the original attribute scores. Each disturbance term was randomly drawn from a normal distribution with zero mean and variance equal to five percent of the corresponding original attribute score.

(3) The number of known shopping centres \( N \) was determined by drawing a random number from a normal distribution with mean 7 and variance 2. The distribution of the number of known shopping centres is given in table 2.

(4) The actual known shopping centres were determined by using

\[
INF_i = \exp(-100/X_{i1} - 0.3X_{i3}), \quad \text{where}
\]

\( INF_i \) is an information score of alternative \( i \),

\( X_{ik} \) is the perceived score of alternative \( i \) on attribute \( k \) \((k = 1: \text{floorspace}; k = 3: \text{distance})\).

The shopping centres with the \( N \) highest \( INF \)-value were assumed to be known.

(5) Each consumer was assumed to choose 1,000 times one of the known shopping centres. The number of times each known centre was chosen

<table>
<thead>
<tr>
<th>Number of known centres</th>
<th>Number of consumers</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
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<td>9</td>
<td>13</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
</tr>
</tbody>
</table>
was determined as follows. First, the deterministic utility component $V_i$ of each known alternative was calculated by using eq. (3). The used parameter values were 0.01, 0.1 and $-0.1$ for floorspace, price setting and distance between residence and shopping centre, respectively. Next, 1,000 random utility components were generated for each known choice alternative. These numbers were drawn from a multivariate normal distribution with mean 0, variance 1 and covariances $COV_{ij}$. The alternative chosen the first time was determined by adding the first random utility component of each alternative to the corresponding deterministic utility component. The alternative with the highest utility was assumed to be chosen. The alternative chosen the second time was determined by adding the second series of random components to the deterministic components. Again, the alternative with the highest utility was assumed to be chosen. This process was repeated until 1,000 'choices' were made. Finally, the number of times each known shopping centre was chosen was counted.

The substitution data sets were generated by using eqs. (9) and (10) for $COV_{ij}$. To generate the spatial structure data sets, $COV_{ij}$ was calculated by using eqs. (19) and (20). The parameters $\theta$ and $\alpha$ were assumed to be equal to unity, while the parameters $\phi$ and $\gamma$ were set to respectively $-0.5$ and $0.1$. This means that the substitution effects were assumed to be at their maximum ($\theta=1.0$) and that the spatial structure effects were assumed to be maximum agglomeration effects ($\phi = -0.5$). The distances between pairs of shopping centres $[d_{ij}$ in eq. (20)] were measured as the Euclidean distance between the shopping centres plus a disturbance term which was drawn from a normal distribution with zero mean and variance equal to five percent of the Euclidean distance.

The data of the first substitution set and the first spatial structure set contain for each consumer the perceived attribute scores of the known shopping centres and the number of times each of these centres was chosen. In addition, the spatial structure set contains for each consumer the perceived distances between the pairs of known shopping centres.

The second substitution set and the second spatial structure set were generated in the same way as the first data sets, except that it was assumed that a new shopping centre was constructed at coordinate-pair (33, 22), which is close to the central shopping centre. This centre has a relatively large floorspace (70 units) and a price setting score of seven units. It was assumed that a consumer knows the new shopping centre if the information score [eq. (21)] of the new centre is not smaller than the smallest information score of the known existing shopping centres. It appeared that the new shopping centre was known by 86 consumers.

Note that the scores on the first two attributes of the new choice
alternative are rather close to the scores on these attributes of some of the existing shopping centres. Especially for those consumers living at about equal distances to one of these centres and the new centre, substitution effects can affect the number of times the new shopping centre is chosen substantially. Because the new shopping centre was located rather close to the central shopping centre, spatial structure effects can especially affect the choice behaviour of consumers who are familiar with both the new centre and the central shopping centre.

4. Model calibration and prediction of choice behaviour

In this section, the calibration results for the selected choice models are reported. By using the simulated data sets described in the previous section, it is possible to compare the performance of the selected choice models, and especially to determine to what extent the behaviour of the substitution probit model proposed by Kamakura and Srivastava (1984) and its spatial structure analogy can be approximated by other models.

The parameter values of the choice models were estimated by using the computer package 'CALDIS' [Borgers (1985)], which is an extended version of 'CHOMP' [Daganzo and Schoenfeld (1978)]. CALDIS optimizes the log likelihood function, adjusted for replications [see McFadden (1974)] by using a gradient search method and/or a sequential linear search method. First, the gradient search method was used to find the best parameter values. However, a disadvantage of this method is that it may fail to converge when some of the true parameter values lie near their (theoretical) lower or upper bound. Another disadvantage of this search method is that it may converge at a suboptimal point in the parameter space. Therefore, when necessary, the sequential linear search method which is slower, but less characterized by these disadvantages, was used to finish the search process. The choice probabilities for the probit models were approximated by the Clark (1961) method. All substitution and spatial structure parameters were constrained to their theoretical domain in the parameter space.

The correspondence between the simulated choice data and the choice data predicted by each calibrated model was determined by using two goodness-of-fit measures, based on the sum of absolute differences (SAD) between the simulated and predicted data and the log likelihood (LL) respectively. The measures are scaled as follows:

\[
\%SAD = \left[ \frac{(SAD_q - SAD)}{SAD_{\text{max}} - SAD_q} \right] \times 100\%,
\]

\[
\%LL = \left[ \frac{(LL - LL_q)}{LL_{\text{max}} - LL_q} \right] \times 100%.
\]

The goodness-of-fit measures subscripted by ‘q’ were calculated by assuming
that the probability of a consumer choosing one of the known shopping centres is $1/N$, where $N$ is the number of shopping centres the consumer knows. The measures indicated by 'x' were determined by assuming that the simulated and predicted data correspond exactly (thus $SAD_x = 0$). When $\%SAD$ and $\%LL$ are equal to 0%, the model does not produce better predictions than assuming equal shares for all known choice alternatives. When the predicted data corresponds exactly to the simulated data, $\%SAD$ and $\%LL$ are both equal to 100%.

For each of the calibrated choice models, the correspondence between the predicted data and the simulated data after the introduction of the new choice alternative was also determined.

The similarity measure included in the Meyer and Eagle model has not been determined by using Pearson's product moment correlation coefficient, but by using the following more sensitive measure:

$$R_i = \left[ \sum_j \sum_k |X'_{ik} - X_{jk}| \right]/N*K,$$

where

$$X'_{ik} = X_{ik}/X_{ik}^{max},$$

$X_{ik}^{max}$ is the maximum score on attribute $k$ over the available choice alternatives,

$K$ is the number of attributes,

$N$ is the number of available choice alternatives.

For Hausman and Wise's perceptual interdependence model, the $\text{VAR}(e^*)$-terms were assumed to be zero to enable the model to account for maximum substitution effects. Homoscedasticity was assumed for the Kamakura and Srivastava model: all variances were set to unity.

4.1. Substitution effects

The multinominal logit model, the substitution models and the spatial structure models were estimated given the first substitution set which was generated by the simulation. The data of the first substitution set and the data of the second substitution set were predicted by the calibrated models. The goodness-of-fit measures $\%SAD$ and $\%LL$ are shown in table 3. Note that both measures yield about the same rank orderings of the models. Therefore, the evaluation of the performance of the choice models is based mainly on the more sensitive scaled sum of absolute differences ($\%SAD$).

The first four models, the multinominal logit model and the extended substitution logit models show similar results. The maximum difference between the worst (multinominal logit) and best (Borgers and Timmermans'
Table 3
Results of model calibration on the substitution set.

<table>
<thead>
<tr>
<th>Model</th>
<th>Estimation set</th>
<th>Prediction set</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>%SAD %LL</td>
<td>%SAD %LL</td>
</tr>
<tr>
<td>Multinomial logit</td>
<td>86.47 97.64</td>
<td>82.29 97.17</td>
</tr>
<tr>
<td>Substitution models</td>
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<tr>
<td>Meyer and Eagle</td>
<td>87.64 98.04</td>
<td>87.61 97.84</td>
</tr>
<tr>
<td>Batsell</td>
<td>87.30 97.92</td>
<td>86.63 97.69</td>
</tr>
<tr>
<td>Borgers and Timmermans</td>
<td>88.35 98.22</td>
<td>87.50 97.97</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z)</td>
<td>74.95 91.13</td>
<td>74.97 91.39</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z²)</td>
<td>69.60 84.77</td>
<td>69.27 85.25</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z³)</td>
<td>59.37 72.01</td>
<td>57.82 72.19</td>
</tr>
<tr>
<td>Hausman and Wise</td>
<td>77.48 85.79</td>
<td>74.31 81.53</td>
</tr>
<tr>
<td>Kamakura and Srivastava</td>
<td>95.82 99.70</td>
<td>95.68 99.56</td>
</tr>
<tr>
<td>Spatial structure models</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spatial structure logit</td>
<td>86.56 97.65</td>
<td>85.41 97.20</td>
</tr>
<tr>
<td>Spatial structure probit</td>
<td>87.78 97.64</td>
<td>87.19 97.40</td>
</tr>
</tbody>
</table>

substitution model) of these models in terms of the scaled sum of absolute differences is about two percent. These models perform less well than Kamakura and Srivastava's probit model. However, the difference is relatively small: about eight percent. Table 3 also demonstrates that the scaled sum of absolute differences decreases about one percent for these models when the choice probabilities which result after introducing the new shopping centre are predicted. This is considerably more than the decrease in %SAD of the Kamakura and Srivastava model.

The transformations proposed by Cooper and Nakanishi lead to disappointing results. These transformations of the attribute scores are apparently too rigorous to approximate the assumed utility values of the choice alternatives. Table 3 evidences that the more rigorous the transformation, the less the percentage scaled sum of absolute differences. Using the zeta-squared transformation resulted even in a wrong sign for the price setting parameter. Note that according to the scaled log-likelihood, the performance of these models increases when predicting the simulated data after introducing the new shopping centre.

The perceptual interdependence probit model by Hausman and Wise is also unable to reproduce the simulated data well. This may be caused by the fact that the structure of its variance-covariance matrix is quite different from the structure of this matrix for the Kamakura and Srivastava model: the Kamakura and Srivastava model assumes homoscedasticity while the variances of the error terms in the Hausman and Wise model may differ.
substantially. Another reason may be that the Clark method to approximate the choice probabilities is less accurate when the variances in the variance-covariance matrix differ.

The performance of the probit model proposed by Kamakura and Srivastava is very good. The scaled sum of absolute errors is almost 96 percent. This good performance hardly reduces when the choice probabilities after introducing the new choice alternative are predicted. The scaled sum of absolute differences decreases only 0.14 percent.

Compared with the Cooper and Nakanishi transformation models and the perceptual interdependence model, the performance of both spatial structure models is not bad at all. According to the scaled sum of absolute differences, the spatial structure logit model performs equally well as the conventional MNL model while the spatial structure probit model performs as well as the extended substitution logit models.

Another criterion to judge the performance of the choice models is to compare the predicted total shares of the new choice alternative with its simulated total share. These figures are shown in table 4, which contains the predicted and simulated total shares in percentages and the predicted shares as an index figure of the simulated share. The simulated total share for the new choice alternative is reproduced very well by the Kamakura and Srivastava model, while the models using a Cooper and Nakanishi transformation, and especially the Hausman and Wise model give rather bad

<table>
<thead>
<tr>
<th>Model</th>
<th>Percentage</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multinomial logit</td>
<td>8.2</td>
<td>116.7</td>
</tr>
<tr>
<td><strong>Substitution models</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Meyer and Eagle</td>
<td>7.5</td>
<td>106.9</td>
</tr>
<tr>
<td>Batsell</td>
<td>7.7</td>
<td>109.2</td>
</tr>
<tr>
<td>Borgers and Timmermans</td>
<td>7.9</td>
<td>111.3</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z)</td>
<td>8.6</td>
<td>121.7</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z²)</td>
<td>8.2</td>
<td>116.0</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z³)</td>
<td>8.6</td>
<td>121.4</td>
</tr>
<tr>
<td>Hausman and Wise</td>
<td>4.0</td>
<td>57.2</td>
</tr>
<tr>
<td>Kamakura and Srivastava</td>
<td>7.3</td>
<td>103.0</td>
</tr>
<tr>
<td><strong>Spatial structure models</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spatial structure logit</td>
<td>8.2</td>
<td>116.9</td>
</tr>
<tr>
<td>Spatial structure probit</td>
<td>6.8</td>
<td>96.1</td>
</tr>
<tr>
<td>Simulated total share</td>
<td>7.1</td>
<td>100.0</td>
</tr>
</tbody>
</table>
predictions of the simulated total share. Note again that the predictions of the spatial structure models are closer to the simulated share than the predictions by some of the substitution models.

4.2. Spatial structure effects

After calibrating the choice models on the simulated substitution set, the models were calibrated on the simulated spatial structure data set. The goodness-of-fit measures for the predictions before and after the introduction of the new shopping centre and the predicted total shares for the new shopping centre are summarized in tables 5 and 6.

These tables show that the multinomial logit model and the extended substitution logit models perform almost equally well. Again, the models using a Cooper and Nakanishi transformation and the Hausman and Wise model give disappointing results. Like the previous calibration session, the more rigorous the Cooper and Nakanishi transformation, the worse the performance of the model. The substitution model proposed by Kamakura and Srivastava outperforms each of the other substitution models.

Because the models are calibrated on the spatial structure data set, both spatial structure models are expected to perform well. However, the results of the spatial structure logit model are not as good as the results of the Kamakura and Srivastava substitution model, although the scaled sum of absolute differences by the spatial structure logit model decreases less than the scaled sum of absolute differences by the Kamakura and Srivastava

Table 5

Results of model calibration on the spatial structure set.

<table>
<thead>
<tr>
<th>Model</th>
<th>Estimation set</th>
<th>Prediction set</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>%SAD</td>
<td>%LL</td>
</tr>
<tr>
<td>Multinomial logit</td>
<td>91.59</td>
<td>98.65</td>
</tr>
<tr>
<td>Substitution models</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Meyer and Eagle</td>
<td>91.58</td>
<td>98.64</td>
</tr>
<tr>
<td>Batsell</td>
<td>91.59</td>
<td>98.55</td>
</tr>
<tr>
<td>Borgers and Timmermans</td>
<td>91.72</td>
<td>98.67</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z)</td>
<td>74.35</td>
<td>90.94</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z²)</td>
<td>71.11</td>
<td>87.25</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z⁴)</td>
<td>67.83</td>
<td>80.65</td>
</tr>
<tr>
<td>Hausman and Wise</td>
<td>68.57</td>
<td>78.32</td>
</tr>
<tr>
<td>Kamakura and Srivastava</td>
<td>95.07</td>
<td>99.56</td>
</tr>
<tr>
<td>Spatial structure models</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spatial structure logit</td>
<td>91.88</td>
<td>98.82</td>
</tr>
<tr>
<td>Spatial structure probit</td>
<td>98.24</td>
<td>99.91</td>
</tr>
</tbody>
</table>
A. Borgers and H. Timmermans, Choice model specification

Table 6
Predicted total share (as percentage and as index figure of simulated share) for the new shopping centre for the spatial structure set.

<table>
<thead>
<tr>
<th>Model</th>
<th>Percentage</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multinomial logit</td>
<td>8.0</td>
<td>86.8</td>
</tr>
<tr>
<td><strong>Substitution models</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Meyer and Eagle</td>
<td>8.0</td>
<td>86.8</td>
</tr>
<tr>
<td>Batsell</td>
<td>7.7</td>
<td>83.4</td>
</tr>
<tr>
<td>Borgers and Timmermans</td>
<td>7.9</td>
<td>85.8</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z)</td>
<td>8.7</td>
<td>94.6</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z)</td>
<td>8.3</td>
<td>89.6</td>
</tr>
<tr>
<td>Cooper and Nakanishi (Z²)</td>
<td>8.5</td>
<td>91.6</td>
</tr>
<tr>
<td>Hausman and Wise</td>
<td>4.0</td>
<td>43.6</td>
</tr>
<tr>
<td>Kamakura and Srivastava</td>
<td>8.4</td>
<td>90.4</td>
</tr>
<tr>
<td><strong>Spatial structure models</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Borgers and Timmermans logit</td>
<td>8.4</td>
<td>90.5</td>
</tr>
<tr>
<td>Borgers and Timmermans probit</td>
<td>9.3</td>
<td>101.1</td>
</tr>
<tr>
<td>Simulated total share</td>
<td>100.0</td>
<td></td>
</tr>
</tbody>
</table>

substitution model after the introduction of the new choice alternative. Calibrating the model which was used to generate the spatial structure data sets gives very good results. The scaled sum of absolute differences before and after the introduction of the new shopping centre is very high and the predicted total share for the new shopping centre is quite similar to the simulated total share for this shopping centre.

5. Summary and conclusions

In this study, a simulation experiment was conducted to generate data sets incorporating substitution or spatial structure effects. These effects on choice behaviour depend on two matters. First, the decision makers must be sensitive to these effects. Second, the characteristics of the available choice alternatives must enable the substitution or spatial structure effects to play a role in the choice behaviour of individuals. In this study, the decision makers were assumed to be maximally sensitive to substitution or spatial structure effects. The spatial structure effects were assumed to appear as agglomeration effects. The characteristics of the choice alternatives (shopping centres) were determined in such a way that substitution effects are not able to be at their maximum, however, the characteristics of particular pairs of choice alternatives are closer to each other than the characteristics of other pairs of alternatives. Further, two choice alternatives were never located so close to
each other that agglomeration effects can be at their maximum, but some pairs of choice alternatives are located closer to each other than other pairs.

Four data sets were generated by means of a simulation. The first two data sets were generated by assuming the existence of substitution effects. The choice data were generated using a probit model proposed by Kamakura and Srivastava (1984). Several models were estimated using the first of these data sets. The second data set, which contains observations after introducing a new choice alternative, was used to determine the external validity of the calibrated models. The calibrated choice models were compared in terms of their ability to reproduce the generated data. Some main conclusions may be drawn from this experiment. First, the calibrated probit model by Kamakura and Srivastava reproduces its 'own' data very well, while another probit model proposed by Hauseman and Wise (1978) gives a bad reproduction of the simulated data. Second, although Kamakura and Srivastava's model performs better, the conventional multinomial logit model is still able to produce a reasonable fit to the simulated data. This result may be taken as an indication of the robustness of the MNL model. Third, some extended logit models which are able to account for substitution effects reproduce the simulated data marginally better than the conventional logit model. Further, the use of the Cooper and Nakanishi attribute score transformations in the conventional logit model leads to unsatisfactory results. Finally, two spatial structure models, an extended logit model and a multinomial probit model, which are not able to account for substitution effects, fit the data at least as well as the MNL model.

The last two data sets were generated by assuming the existence of agglomeration effects. A spatial structure probit model proposed by Borgers and Timmermans (1985a, b) was used to generate these two data sets. Again, the first of these sets was used to calibrate several choice models while the second set was used to determine the performance of the calibrated models after introducing a new choice alternative. The main conclusions which can be drawn from this experiment are similar to the main conclusions of the experiment with the substitution effects. As expected, the spatial structure probit model reproduces the data very well. Again, the MNL model seems to be rather robust, while the spatial structure logit model performs a little better than the MNL model. The substitution logit models reproduce the data as well as the MNL model and the models with a Cooper and Nakanishi transformation give unsatisfactory results. In contrast to the Kamakura and Srivastava model, the perceptual interdependence model is also unable to approximate the simulated data.

Given the results of the experiments, it can be concluded that the multinomial logit model and extensions of this model seem to be robust enough to reproduce the simulated data, which was generated by a more complex (and computationally more burdensome) probit model, reasonably
well. This conclusion may not be drawn for models including a Cooper and Nakanishi attribute score transformation or the probit model proposed by Hausman and Wise, which is not to say that the latter choice models are bad models in general.

Thus, it seems that although the more sophisticated probit model performs better whenever substitution or spatial structure effects are present in the observed data, not very much may be gained by using this complex model instead of the conventional MNL model or an extended MNL model in terms of predictive ability. Considering the fact that estimating a probit model requires considerably more computing time than estimating a logit model, this conclusion is very important in an application context. On the other hand, this conclusion of course applies to the prediction of the total spatial system while the total share for any single choice alternative predicted by the MNL model may differ considerably more from the simulated total shares than the total shares predicted by the probit model. Especially in a planning context this may be decisive. It should be emphasized that this conclusion is based only on some simulation experiments. Hence, analysis such as conducted in the present study should be repeated and augmented with empirical studies. The authors hope to report on such empirical analyses in the near future.

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