Spatial microsimulation: a practical introduction

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Contents

Chapter 1

Preface

The trigger for this book's creation was a two day course, An Introduction to Spatial Microsimulation with R, held at the University of Leeds in the spring of 2014. Based on the high demand before the course and feedback from participants taking part, it seemed there was a definite need for more practical teaching material on spatial microsimulation than was available at the time: many people had read the literature and had a good idea about the problem that they wanted to harness the method to solve. Yet the majority were dissatisfied with the *practical* content of existing work, or lack thereof.

This book is for all those struggling to find material clearly and succinctly explaining how to implement spatial microsimulation on their own datasets.

The underlying motivations for this work go much deeper and are best understood with reference to my own experience of trying to learn spatial microsimulation. I, like many PhD students and researchers, was tasked with implementing the method when it was almost completely new to me. I had barely heard of the method, let alone understood the methodology. The first stage was to read up on what spatial microsimulation actually was: in this area I was fortunate enough to have good guidance from my supervisor Dimitris Ballas, who pointed me towards an accessible introduction to spatial microsimulation commissioned by the Joseph Roundtree Foundation (**?**). Without this text, I'd have been even more bewildered; overcoming this bewilderment is a central aim of this course. It will not demonstrate how, exactly, to apply the method to your own datasets, but it will provide strong foundations that should enable the method to be applied to almost any combination of individual and aggregate level datasets, provided suitable shared variables between the two. As emphasised in the closing chapter of the book, it is the responsibility of the researcher to ensure that the method is applied in a rigorous and ethical way: this cannot be taught, although the extensive CakeMap example will demonstrate how the method can be used in rather absurd ways.

In addition to good guidance towards introductory reading, another major benefit I had was having Malcolm Campbell as my predecessor. Malcolm provided a huge amount of support during the early phase of my PhD and shared the entirety of the R code he developed to perform spatial microsimulation on his Scottish health data. Not only was the code invaluable to my efforts to build a spatial microsimulation model in R (some of the code in the book is probably his at some level), his example of collaboration and code sharing was truly inspirational. Thus this book owes as much to Malcolm as to anyone else and its free distribution under the Creative Commons license is partly a result of his generosity in sharing code and enthusiasm of teaching tricky statistical techniques.

Chapter 2

What is spatial microsimulation?

Spatial microsimulation is shrouded by an unnecessary mystery, and this is worsened by much of the literature on the subject. Most academic papers and even some textbooks about spatial microsimulation lack reproducible examples. In today's age of fast Internet connections, open access datasets and free software, things need not be this way. One could argue that the lack of reproducibility in spatial microsimulation is damaging to the growth and credibility of the field.

To those doubting the value of this practical approach, I ask the following questions: If only a small community of researchers hold the majority of the code needed to perform spatial microsimulation, how can the technique spread rapidly to other applications? If every PhD student undertaking spatial microsimulation must start from scratch, how are the methods going to be refined and improved in a systematic fashion? Most importantly, if the results of most spatial microsimulation research is not reproducible — as is currently the case — how can we trust them?

This final point is critical not only to spatial microsimulation but the disciplines of which it is part. Reproducibility is a prerequisite of falsifiability — if the method underlying a result cannot be replicated by others, how can the finding possibly be falsified? Moreover, the argument continues, any knowledge or theory can only claim to enter the realm of 'science' if it cannot be falsified. Because it is impossible to prove any proposition in every and all cases, the only reliable test we can apply is whether or not it can be *disproved*: falsified via a contradictory finding. This is how scientific progress is made (**?**). By writing non-reproducible research, researchers may inadvertently damage the disciplines in which they work.

Despite and because of these philosophical antecedents, the course is unashamedly practical. The aim is simple: to provide an accessible yet deep foundation in spatial microsimulation. This involves both *understanding* and *implementation* of the technique. Following the 'learning by doing' ethic, the former can best be attained through the latter: spatial microsimulation need not be an abstract process that one simply reads about. It can be practical tool used by anyone with the know-how. As **?**, xxii put it regarding R, "the best way to learn is to experiment" and the same applies to spatial microsimulation.

The examples presented below were developed during a PhD project in the energy costs of commuting. Although some of the code and most of the descriptive text has been rewritten since then, many of the ideas and methods are described in more detail in the resulting thesis.

Chapter 3

Applications

Chapter 4

Spatial microsimulation with R

4.1 Why R?

Software decisions have a major impact on the model's flexibility, efficiency, reproducibility and ease of coding. **?**, p. 153 observed that "little attention is paid to the choice of programming language used." This appears to be as true now as it was then: software is rarely discussed in spatial microsimulation papers. In my own spatial microsimulation research, a conscious decision was made early on to use R, with impacts on model features, analysis and even design. It is thus worth understanding the tool a little before we begin to use it. The theory is discussed in section 4.2

The world is awash with computer programming languages and many of these are general purpose and 'Turing complete', meaning they could, with sufficient effort, perform spatial microsimulation. So why would one chose R? The most important criteria of evaluation include flexibility, speed of processing and, most importantly, ease and speed of writing code. R excels in each of these areas, especially the final one: it is possible to say a lot in R in few lines of code. Further are provided by **?**:

- "a public-domain implementation of the widely-regarded S statistical language; R/S is the de facto standard among professional statisticians
- comparable, and often superior, in power to commercial products in most senses
- available for Windows, Macs, Linux
- in addition to enabling statistical operations, it's a general programming language, so that you can automate your analyses and create new functions

- object-oriented and functional programming structure
- your data sets are saved between sessions, so you don't have to reload each time
- open-software nature means its easy to get help from the user community"

4.2 IPF theory: a worked example

IPF is a simple statistical procedure, "in which cell counts in a contingency table containing the sample observations are scaled to be consistent with various externally given population marginals" (**?**). In other words, and in the context of *spatial* microsimulation, IPF produces maximum likelihood estimates for the frequency with which people appear in different areas. The method is also known as 'matrix raking' or the RAS algorithm, and has been described as one particular instance of a more general procedure of 'entropy maximisation' (**?**). The mathematical properties of IPF are described in earlier papers (e.g. **?**). A practical example of the procedure can be found in **?**, who provides an implementation in Microsoft Excel.

The simple example below demonstrates how IPF works. Table 4.1 describes a hypothetical microdataset comprising 5 individuals, who are defined by two constraint variables: age and sex. Each has two categories. Table 4.2 contains aggregated data for a hypothetical area. Table 4.3 illustrates this table in a different form, which shows the unknown links between age and sex in the aggregate data.

Table 4.1: A hypothetical input microdata set (the original weights set to one). The bold value is used subsequently for illustrative purposes.

Individual	Sex	Age-group	Weight
1	Male	Over-50	1
2	Male	Over-50	1
3	Male	Under-50	**1**
4	Female	Over-50	1
5	Female	Under-50	1

Table 4.4 presents the hypothetical microdata in aggregated form, that can be compared directly to Table 4.3.

IPF readjusts the weights of the hypothetical individuals so that their add up to the totals given in Table 4.3.

Table 4.2: Hypothetical small area constraints data (s).

Constraint ⇒	i		j	
Category ⇒	i_1	i_2	j_1	j_2
Area ⇓	Under-50	Over-50	Male	Female
1	8	4	6	6

Table 4.3: Small area constraints expressed as marginal totals, and the cell values to be estimated.

Marginal totals		j		
	Age/sex	Male	Female	T
i	Under-50	**?**	?	8
	Over-50	?	?	4
	T	6	6	12

Table 4.4: The aggregated results of the weighted microdata set ($m(1)$). Note, these values depend on the weights allocated in Table 4.1 and therefore change after each iteration

Marginal totals		j		
	Age/sex	Male	Female	T
i	Under-50	**1**	1	2
	Over-50	2	1	3
	T	3	2	5

The weights are multiplying by the marginal totals taken from Table 4.2 and then divided by the respective marginal total in 4.4. This is done one constraint at a time. This is described in eq. (4.1) for constraint i (age in this case):

$$w(n+1)_{ij} = \frac{w(n)_{ij} \times sT_i}{mT(n)_i} \tag{4.1}$$

where $w(n+1)_{ij}$ is the new weight for individuals with characteristics i (age, in this case), and j (sex), $w(n)_{ij}$ is the original weight for individuals with these characteristics, sT_i is element marginal total of the small area constraint, s (Table 4.2) and $mT(n)_i$ is the marginal total of category j of the aggregated results of the weighted microdata, m (Table 4.4). n represents the iteration number. Although the marginal totals of s are known, its cell values are unknown. Thus, IPF estimates the interaction (or cross-tabulation) between constraint variables. (Follow the emboldened values in the tables to see how the new weight of individual 3 is calculated for the sex constraint.) Table 4.5 illustrates the weights that result. Notice that the sum of the weights is equal to the total population, from the constraint variables.

Table 4.5: Reweighting the hypothetical microdataset in order to fit Table 4.2.

Individual	Sex	age-group	Weight	New weight, w(2)
1	Male	Over-50	1	$1 \times 4/3 = \frac{4}{3}$
2	Male	Over-50	1	$1 \times 4/3 = \frac{4}{3}$
3	Male	Under-50	1	$\mathbf{1} \times \mathbf{8/2} = 4$
4	Female	Over-50	1	$1 \times 4/3 = \frac{4}{3}$
5	Female	Under-50	1	$1 \times 8/2 = 4$

After the individual level data have been re-aggregated (table 4.6), the next stage is to repeat eq. (4.1) for the age constraint to generate a third set of weights, by replacing the i in sT_i and $mT(n)_i$ with j and incrementing the value of n:

$$w(3)_{ij} = \frac{w(2)_{ij} \times sT_j}{mT(2)_j} \tag{4.2}$$

To test your understanding of IPF, apply eq. (4.2) to the information above and that presented in table 4.6. This should result in the following vector of new weights, for individuals 1 to 5. Calculate the correct values and pencil them in in place of the question marks. One 'sanity' check of your method here is whether the sum of these weights is still equal to twelve.

$$w(3) = (\frac{6}{5}, \frac{?}{?}, \frac{18}{5}, \frac{?}{?}, \frac{9}{2}) \tag{4.3}$$

Notice also that after each iteration the fit between the marginal totals of m and s improves. The total absolute error (TAE) improves between $m(1)$ to $m(2)$, falling from 14 to 6 in table 4.4 and table 4.6 above. TAE for $m(3)$ (not shown, but calculated by aggregating $w(3)$) improves even more, to 1.3. This number would eventually converge to 0 through subsequent iterations, as there are no empty cells in the input microdataset; a defining feature of IPF.

The above process, when applied to more categories (e.g. socio-economic class) and repeated iteratively until a satisfactory convergence occurs, results in a series of weighted microdatasets, one for each of the small areas

Table 4.6: The aggregated results of the weighted micro-data set after constraining for age ($m(2)$).

Marginal totals		i		
	Age/sex	Male	Female	T
j	Under-50	4	4	8
	Over-50	$\frac{8}{3}$	$\frac{4}{3}$	4
	T	$6\frac{2}{3}$	$5\frac{1}{3}$	12

being simulated. This allows for the estimation of variables whose values are not known at the local level (e.g. income). An issue with the results of IPF (absent from combinatorial optimisation methods), however, is that it results in non-integer weights: fractions of individuals appear in simulated areas. As described in the introduction, this is not ideal for certain applications. Integer weights allow the results of spatial microsimulation to be further processed using dynamic microsimulation and agent based modelling techniques (**?**).

Spatial microsimulation can also provide insight into the likely distribution of individual level variables about which only geographically aggregated statistics have been made available. An issue with the results of IPF (absent from combinatorial optimisation methods), however, is that it results in non-integer weights: fractions of individuals appear in simulated areas.

4.3 Implementing IPF in R

The above example is best undertaken by hand, probably with a pen and paper to gain an understanding of IPF, before the process is automated for larger datasets. This section explains how the IPF algorithm described above was implemented in R, using a slightly more complex example. (?).[1]

Loading in the data

In the full model the input datasets are stored as .csv files, one for each constraint and one for the input microdata, and read in with the command `read.csv`. For the purposes of understanding how the model works, the dataset is read line by line, following the example above. The following code creates example datasets, based on the same hypothetical survey of 5 individuals described above, and 5 small areas. The spatial microsimulation model will select individuals based on age and sex and mode of transport (mode of transport is also used on the larger online

[1]This tutorial is available from Rpubs, a site dedicated to publishing R analyses that are reproducible. It uses the RMarkdown mark-up language, which enables R code to be run and presented within documents. See http://rpubs.com/RobinLovelace/5089 .

example described in footnote 1). For consistency with the (larger) model used for the paper, the individual level data will be referred to as USd (Understanding Society dataset) and the geographic data as all.msim (for all constraint variables). The code to read-in the individual level data are presented in code sample 4.1. When called, the data are then displayed as a table (see listing 4.2). The

Listing 4.1: Manual input of individual level data in R

```
# Read in the data in long form (normaly read.table()
c.names <- c("id", "age", "sex")
USd <- c(        1, 59, "m",
                 2, 54, "m",
                 3, 35, "m",
                 4, 73, "f",
                 5, 49, "f")
USd <- matrix(USd, nrow = 5, byrow = T) # Long data i
USd <- data.frame(USd) # Convert this into a datafram
names(USd) <- c.names # Add correct column names
USd$age <- as.numeric(levels(USd$age)[USd$age]) # Age
```

same procedure applies to the geographical data (listing 4.3).

IPF relies on the assumption that all constraint variables will contain the same number of people. This is

Listing 4.2: Output of the USd data frame

```
USd # Show the data frame in R
##   id age sex
## 1  1  59   m
## 2  2  54   m
## 3  3  35   m
## 4  4  73   f
## 5  5  49   f
```

logical (how can there be more people classified by age than by sex?) but can cause problems for constraint variables that use only a subset of the total population, such as those who responded to questions on travel to work. To overcome this problem, it is possible to normalise the constraint variables, setting the total for each to the one that has the most reliable total population. This worked example simply checks whether or not they are (listing 4.4).

Reweighting the survey dataset

Iterative proportional fitting determines the weight allocated to each individual for each zone to best match the geographically aggregated data. A weight matrix is therefore created, with rows corresponding to individuals and columns to zones, as described in section 4.2. In R, this, and the creation of the aggregated results matrix, is done with code presented in listing 4.5).[2]

It is important to note that in real survey data, the variables are not always neatly categorised into the same bins as the levels of the aggregate data. Age, for example can be classified in many different ways. Also, a wide form is useful for subsequent steps. Therefore, it is necessary to convert the 'thin' survey dataset into a wider form, by converting a single column such as age or sex into multiple columns corresponding to the number of categories. Sometimes the cut-off points of the categories can be decided (as with age), or categories can be merged (when many different NA options are available, for example). The code that performs this important process for our example dataset is presented in listing 4.6.

Another important step shown in section 4.2 was that of converting the 'long' survey dataset into a form that can be compared directly with the aggregated constraint variables. Listing 4.7 shows how this is done in R, and the code needed to view the results. (Notice that the first row of all.msim is the same as those displayed in table 4.2)

With the data loaded and processed into comparable

[2]In subsequent versions of the model, single, multi-dimensional weight and aggregated result matrices are used, to reduce the length of the scripts.

formats, one is in a position to start comparing how well our individual level survey dataset fits with the aggregate constraints (see listing 4.7). Note that for USd.agg, the results are the same for every zone, as each individual has a weight of 1 for every zone. Note also the very poor fit between the variables at the aggregate level, as illustrated by poor correlation between the constraint and microdata variables (r = 0.05), and a plot of the fit presented in fig. 4.1. The next stage is to apply the first constraint, to adjust the weights of each individual so they match the age constraints (listing 4.8 — note that the top row USd.agg1 is the same as table 4.6). After this operation, the fit between the constraint variables and the aggregated microdata are far better (r = 0.67), but there is still a large degree of error (fig. 4.2).

We will perform the same checks after each constraint to ensure our model is improving. To see how the weights change for each individual for each area, one simply types `weights1`, for constraint 1 (listing 4.9). Note that the first column of weights 1 is the same as table 4.2.

Listing 4.9: The new weight matrix. Previously all weights were set to one.

```
##         [,1]  [,2]  [,3]  [,4] [,5]
## [1,] 1.333 2.667 1.333 1.333  1.0
## [2,] 1.333 2.667 1.333 1.333  1.0
## [3,] 4.000 1.000 3.500 2.500  3.5
## [4,] 1.333 2.667 1.333 1.333  1.0
## [5,] 4.000 1.000 3.500 2.500  3.5
```

To further improve the fit, one next constrains by the second aggregate constraint: sex (listing 4.10). To check that our implementation in R produces the same results as the hand-calculated example, the resulting weights where queried. As shown by `weights3[,1]`, these are the same as those calculated for $w(3)$ above.

The model fit improves greatly after constraining for sex (r = 0.992). However, to ensure perfect fit more iterations are needed. Iterating just once more, as done on the online version of this section[3] results in a fit that is virtually perfect (fig. 4.3). More iterations are needed for larger datasets with more constraints to converge.

The worked code example in this section is replicable. If all the code snippets are entered, in order, the results should be the same on any computer running R. There is great scope for taking the analysis further: some further tests and plots are presented on the on-line versions of this section. The simplest case is contained in Rpubs document 6193 and a more complex case (with three constraints) can be found in Rpubs document 5089. The preliminary

[3]See rpubs.com/RobinLovelace/6193

checks done on this code are important to ensure the model is understood at all times and is working correctly. More systematic methods for model checking are the topic of the following section.

Listing 4.3: Geographic data input

```
 category.labels <- c("16-49", "50+" # Age constraint
                ,"m", "f" # Sex constraint
                # more constraints could go here
                )
all.msim <- c(  8, 4,    6, 6,
# Original aggregate data
                2, 8,    4, 6,
# Elderly
                7, 4,    3, 8,
# Female dominated
                5, 4,    7, 2,
# Male dominated
                7, 3,    6, 4    # Young
                )
all.msim <- matrix(all.msim, nrow = 5, byrow = T)
all.msim <- data.frame(all.msim) # Convert to datafra
names(all.msim) <- category.labels # Add correct colu
```

Listing 4.4: R code to check the constrain populations match

```
 # Check totals for each constraint match
rowSums(all.msim[,1:2]) # Age constraint
## [1] 12 10 11  9 10
rowSums(all.msim[,3:4]) # Sex constraint
## [1] 12 10 11  9 10

rowSums(all.msim[,1:2]) == rowSums(all.msim[,3:4]
## [1] TRUE TRUE TRUE TRUE TRUE
```

Listing 4.5: Creating arrays of weights in R

```
weights0 <- array(dim=c(nrow(USd),nrow(all.msim))
weights1 <- array(dim=c(nrow(USd),nrow(all.msim))
weights2 <- array(dim=c(nrow(USd),nrow(all.msim))

weights0[,] <- 1 # sets initial weights to 1

USd.agg <- array(dim=c(nrow(all.msim),ncol(all.ms
USd.agg1 <- array(dim=c(nrow(all.msim),ncol(all.m
USd.agg2 <- array(dim=c(nrow(all.msim),ncol(all.m
colnames(USd.agg1) <- category.labels
```

Listing 4.6: R code to convert the survey dataset into binary form

```
USd.cat <- array(rep(0), dim=c(nrow(USd),
                          length(category.labels !=0)

USd.cat[which(USd$age < 50),1] <- 1 # Age, "< 50"
USd.cat[which(USd$age >= 50),2] <- 1 # "50+"
USd.cat[which(USd$sex =="m"),3] <- 1 # Sex constraint
USd.cat[which(USd$sex =="f"),4] <- 1 #"f"
sum(USd.cat) # Should be 10
```

Listing 4.7: R code to aggregate the survey dataset

```
for (i in 1:nrow(all.msim)){ # Loop creating agg
  USd.agg[i,]    <- colSums(USd.cat * weights0[,i]
}

# Test results
USd.agg

##       [,1] [,2] [,3] [,4]
## [1,]     2    3    3    2
## [2,]     2    3    3    2
## [3,]     2    3    3    2
## [4,]     2    3    3    2
## [5,]     2    3    3    2

all.msim

##   16-49 50+ m f
## 1     8   4 6 6
## 2     2   8 4 6
## 3     7   4 3 8
## 4     5   4 7 2
## 5     7   3 6 4

plot(as.vector(as.matrix(all.msim)),
  as.vector(as.matrix(USd.agg)), xlab = "Constrai
    ylab = "Model␣output")
abline(a = 0, b = 1)
```

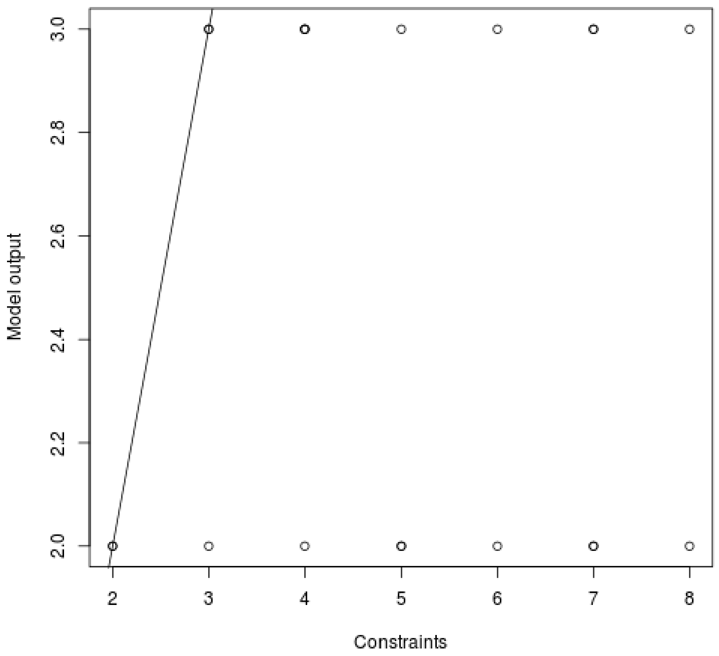


Figure 4.1: Scatter plot of the fit between census and survey data. This plot can be re-created using the plot command in listing 4.7.

Listing 4.8: Reweighting of first constraint and testing of results

```
for (j in 1:nrow(all.msim)) {
 weights1[which(USd$age < 50),j] <- all.msim[j,1]
 weights1[which(USd$age >= 50),j] <- all.msim[j,2
}
# Aggregate the results for each zone
for (i in 1:nrow(all.msim)) {
 USd.agg1[i,] <- colSums(USd.cat * weights0[,i] *
}
# Test results
USd.agg1
##      16-49 50+     m     f
## [1,]     8   4 6.667 5.333
## [2,]     2   8 6.333 3.667
## [3,]     7   4 6.167 4.833
## [4,]     5   4 5.167 3.833
## [5,]     7   3 5.500 4.500

plot(as.vector(as.matrix(all.msim)),
 as.vector(as.matrix(USd.agg1)), xlab = "Constrai
 ylab = "Model␣output")
abline(a = 0, b = 1)
```

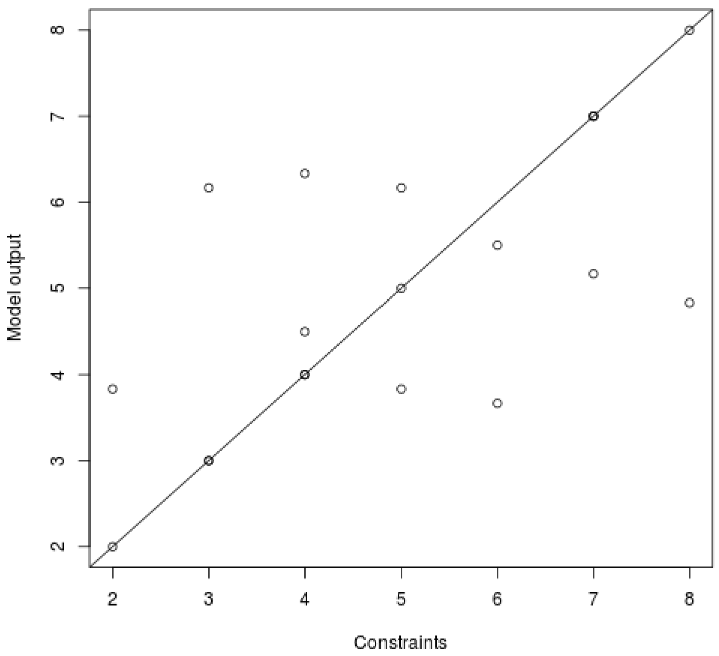


Figure 4.2: Scatter plot showing the fit after constraining by age.

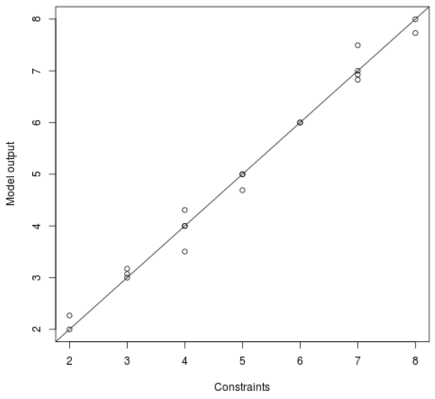
Listing 4.10: Code to constrain the weights by sex

```
for (j in 1:nrow(all.msim)) {
    weights2[which(USd$sex == "m"),j] <-
                    all.msim[j,3]/USd.agg1[j,3]
    weights2[which(USd$sex == "f"),j] <-
                    all.msim[j,4]/USd.agg1[j,4]
}

weights3 <- weights0 * weights1 * weights2
for (i in 1:nrow(all.msim)) {
  USd.agg2[i,] <- colSums(USd.cat * weights3[,i])
}

weights3[,1]

## [1] 1.2 1.2 3.6 1.5 4.5
```



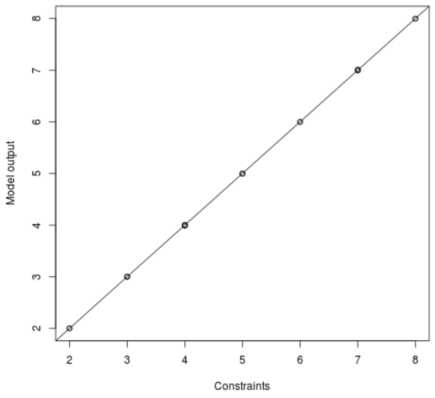


Figure 4.3: Improvement of model fit after constraining by sex (left) and after two complete iterations (right).

Chapter 5

Customising code: a worked example with CakeMap data

Chapter 6

The Flexible Modelling Framework (FMF)

6.1 Model checking and validation

To make an analogy with food safety standards, openness about mistakes is conducive to high standards (**?**). Transparency in model verification is desirable for similar reasons. The two main strategies are 1) comparing the model results with knowledge of how it *should* perform *a-priori* (model checking) and 2) comparison between the model results and empirical data (validation).

6.1.1 Model checking

A proven method of checking that data analysis and processing is working is wide ranging and continual visual exploration of its output (**?**). This strategy has been employed throughout the modelling process, both to gain a better understanding of the behaviour of the underlying R code, and to search for unexpected results. These were often precursors to error identification.

An example of this, that illustrates the utility of ad-hock checks, is the continual plotting of model inputs and outputs to ensure that they make sense. The R commands `summary()` and `plot()` are ideal for this purpose. The former provides basic descriptive statistics; the latter produces a graphical display of the object. Both are *polymorphic*, meaning that command adapts depending on the type of object it has been asked to process (**?**). Thus, to check that the number of people in each age and sex category in the input and output dataset made sense overall, the following command was issued, resulting in the plot illustrated in fig. 6.1:

```
plot(cut(USd$age, breaks=(seq(0,100,20))), USd$se
```

These common-sense methods of data checking may seem overly simplistic to warrant mention. Yet such basic sanity tests are the 'bread-and-butter' of quantitative analysis. They ensure that the data are properly understood (**?**). Had the input data represented in fig. 6.1 contained an equal proportion of people under 20 as over 20, for example, one would know that the input data for commuters was faulty. This approach, whereby major problems are revealed early on in frequent tests, is preferable to waiting until the results of the full spatial microsimulation are analysed. Hours were saved, and understanding of the input datasets was improved.[1]

The basic tenet of spatial microsimulation is that simulated and actual data should match at the aggregate level (**?**). This knowledge led to the continual plotting of census vs simulated results in the early stages of the model construction, and the development of more sophisticated plots (see **??**). Still, the humble scatter plot was used frequently for preliminary analysis. To provide an example, after the model was run for Yorkshire and the Humber region for 20 iterations, I was confident the results were correct: the results had been tested for Sheffield, and everything *seemed* to be working as expected.

[1]The use of the same command to check model output was crucial to the identification of important errors, including a small mistake in the code which led to large errors in the synthetic microdata output for the distance constraint variables.

Knowledge of how model-census fit should look started alarm bells ringing when an imperfect plot was discovered: fig. 6.2 (A) was cause for concern, not only for the low correlation between the two variables (which was still greater than 0.8), but because the direction of the error: the model had *always* overestimated the number of people travelling short distances to work in past runs. This seemed suspicious, and the relationship was plotted for earlier constraints to identify where the problem was variables were plotted. fig. 6.2 (B) was the result of this, after constraining by distance. Something had clearly gone wrong because no people who work from home had been registered in the aggregate output. These issues led to a re-examination of the code contained within the file cats.r. It was found that a faulty placement of an equals sign (such that values "greater than or equal" to 0 were accepted as 0 - 2 km travel to work). The problem was solved, and the model correlation improved as a result (fig. 6.2 (C)).

The two examples described above provided insight into how the model was performing by its own standards. The more challenging stage is to validate the model against factors external to it.

6.1.2 Model validation

Beyond 'typos' or simple conceptual errors in model code, more fundamental questions should be asked of spatial microsimulation models. The validity of the assumptions on which they are built, and the confidence one should have in the results are important. This is especially true of models designed to inform policies which have the potential to influence quality of life. Yet evaluation and 'validation' are problematic for any models that attempt to explain extensive, complex systems such as cities or ecosystems. The urban modelling approach, of which spatial microsimulation of commuters is a subset, has been grappling with this problem since its infancy. Lacking a crystal ball, time-machine or settlements on which controlled experiments can be performed, the difficulty of model evaluation can seem intractable: "only through time can a model be verified in any conventional sense of the word", by comparing the range of projected futures with the reality of future change in hindsight (**?**, p. 15).

Why do urban models pose such a problem? Previously unknown knock-on impacts cannot be ruled out due to the vast number of links between system elements.[2] Rigorous

[2]It is, of course, impossible to know how every resident of an area interacts with every other, let alone predict the future impacts of this interaction, even in the era of ubiquitous digital communications.

real-world testing is usually impossible due to the scale of the system and ethics involved with intervening in peoples' lives for the sake of research. Controlled experiments cannot be performed on real settlements in the same way that experiments can be performed in the physical sciences and, even if two similar settlements could be found on which to apply different interventions, there is no guarantee that all other factors will be held constant throughout the duration of the experiment.

Additional evaluation problems apply to spatial microsimulation models in particular for a number of reasons, including:

- The aggregate values of categorical 'small area' constraint variables are already known from the Census, so should be accurate. Checking the distribution of continuous variables such as age and distance travelled to work against these crude categories is problematic.[3]

[3]For example, if 50% of commuters in a particular area travel 2–5 km to work according to the Census, does that mean that there is a normal distribution of trip distances with the mean focussed on 3.5? Or is it more likely that there is a single large employer located somewhere between 2 and 5 km from the bulk of houses in the area, which accounts for the majority of these jobs and leads to a skewed distribution of home-work distances. In every event, spatial microsimulation will ignore such subtleties and smooth out extreme

- Target variables are not generally known as geographic aggregates. Therefore checking their validity for small areas is difficult: new surveys may be needed.

- Spatial microsimulation results in long lists of individuals for each zone. With thousands of individuals in each zone and hundreds of zones, the datasets can become large and unwieldy.

Regarding the target variables, inaccuracies can be expected because they are determined entirely by their relationships with constraint variables. Also it can be expected these relationships will not remain constant for all places: perhaps in one area the number of female drivers is positively correlated to distance travelled to work, yet there may be a different strength of correlation, or the variables may be unrelated in another.

As mentioned above, validation of target variables is especially problematic due to lack of data. To overcome this problem, two techniques were employed. First, the interaction between constrained variables and unconstrained variables was tested using data from the Census. Second, an additional dataset from the UK's National On-line Manpower Information System (Nomis) was harnessed to

skewness by approximating the national distance trends within each distance bin.

investigate the correlation between unconstrained 'interaction' variables — those composed of two or more constraint variables such as 'female driver'.

The first approach tested the model's ability to simulate income. Although income data are lacking for small areas, Neighbourhood Statistics provides estimates of net and gross household incomes at the MSOA level. For the purposes of this study, equivalised net income was used. The fit between the Neighbourhood Statistics and simulated values are displayed in fig. 6.3.

The results show the microsimulation model could be used to predict income (modelled income), accounting for almost 80% of the variation in the Neighbourhood Statistics data using an ordinary least squares (OLS) regression model. This is impressive, given that the aim of the model is not to simulate income but energy costs of work travel, based on mode, distance, age/sex and class. Of these socio-economic class is the only constraint variable traditionally thought to be closely associated with income. The main problem with the income estimates generated through spatial microsimulation is the small range of estimates simulated: the standard deviation was £1,194 and £3,596 for the simulated and National Statistics data respectively. (Note the differences in the x and y axis scales in fig. 6.3.) This underestimation of variance can be explained because social class, distance and modes of transport are not sufficient to determine the true variability in household incomes. Constraining by car ownership and tenure variables would be likely to improve the fit.

The purpose of this fitting exercise is not so much to provide accurate income estimates at the local level but to evaluate the performance of the spatial microsimulation model. In terms of income, a variable that is unconstrained in the model yet available from the survey data, the spatial microsimulation model has worked well. The results suggest that the values of unconstrained variables will not simply repeat the national average for every small area, but will vary based on how their variation at the national level is related to the constraint variables. In this case, the assumption that the relationships between the target variable (income) and constraint variables at the local level (in Yorkshire and the Humber) are similar to the relationships between these variables at the national level, receives support. How well does the model simulate other target variables such as environmental habits, domestic energy use and levels of deprivation? These are interesting questions that merit further attention based on available data.

The second approach relies on Nomis, which provides cross-tabulations of census variables, for example transport mode by class. The downside is that the data are randomised, as stated at the bottom of each of their small-area census tables: “Figures have been randomly adjusted to avoid the release of confidential data” (this phrase appears in many of Nomis’s tables. One example can be found here: http://www.nomisweb.co.uk/livelinks/4652.xls).

In order to harness Nomis data to test the accuracy of the microsimulation model for calculating, it was first necessary to establish how accurate Nomis data are. How much have Nomis data been randomised, and in what way? This question is relatively easy to answer because of the census variables shared between those published by Nomis and by Casweb at the MSOA level. Scatter plots suggest Nomis data are faithful to the original census results:

From fig. 6.4 it is interesting to note that the correlation decreases for cyclists. This, it was inferred, could represent an increase in the signal-to-noise ratio for variables with small values to a fixed randomising factor. To test this, the errors were plotted for variables with large (car drivers) and small (cyclists) totals. The results indicate that the noise added by randomisation is equal for each variable, regardless of the cell count (fig. 6.5).

The errors seem to be similar, with a range of approximately 70 and a mean of zero. This observation is confirmed by descriptive statistics for each set of errors (standard deviation = 11.01, 9.47; mean = 0.15, 0.23) for car driver and cyclist variables respectively. We can therefore conclude that the error added by randomisation is constant for each variable and this was confirmed by plotting the errors for additional census variables. Q-Q plots — which compare the quantile values of one distribution against another, in this case those of the errors against those of the normal distribution — suggest that the distribution of error is approximately normal.

These exploratory methods provide confidence in the Nomis data, but only for relatively large cell counts (the signal-noise ratio approaches 1:1 as the cell count approaches 20): therefore evaluations based on Nomis data are better suited to cross tabulated categories that have high cell counts, for example car drivers. In our microsimulation model, both gender and mode of transport are constrained, but not simultaneously, so the fit between the Nomis cross-tabulation and the cross-tabulation resulting from our model provides some indication of accuracy. The results are presented in fig. 6.6. Interestingly, the accuracy of this 'partially constrained' simulated target variable appears to be worse than that of the completely unconstrained income variable (compare fig. 6.6 and fig. 6.3). In both cases, the correlation is reasonably strong and positive (0.47 and 0.80 respectively). However, as with the income estimates, the *distribution* of estimates arising from the model is less dispersed than actual data: the standard deviation for the former (0.30) is substantially less than for the latter (0.44). This illustrates the tendency of spatial microsimulation models to underestimate the extent of spatial variation.

6.1.3 Additional validation methods

The methods described above illustrate the techniques used to prevent model errors and ensure that the results were compatible with external data sources. But they only scratch the surface of what is possible in terms of model validation. This section will not go into detail. Its purpose is to draw attention to additional methods that could be conducted as lines of future research and discuss the merits of each. Specifically, the following additional validation methods could (given sufficient resources) be implemented:

- Primary data collection of target variables at the individual level in specific areas to validate the spatial microdata locally.

- Comparing of the spatial microdata over entire region with a survey data that specifies home region of resident.

- Aggregating local model outputs to coarser geographical levels at which cross-tabulated data are available.

- Comparison of mode and distance data with external correlates of personal travel (e.g. MOT data on distance travelled and bus usage data).

Other than the sanity check of age-sex ratios presented in fig. 6.1, the evaluation methods considered above operate at the level of geographically aggregated counts. However, the unique feature of spatial microsimulation is its simulation of individuals. Evaluation techniques should therefore operate at the individual level as well. Because simulation, almost by definition, estimates something that is not otherwise known, it is hard to find reliable individual level data against which the estimates can be evaluated. For this reason individual level surveys could be conducted in a specific area where spatial microdata have been generated. To take one example, a randomised sample of households could be taken in a single ward. Respondents would be asked the mode of travel to work, distance and frequency of trip and other variables. This would allow the model to be evaluated not only in terms of the correlations that it outputs between different categories, but also for the evaluation of the assumptions on which the energy calculations are based.

One of the main advantages of spatial microsimulation over just using aggregated data is that it provides insight into the *distribution* of continuous variables within each zone, rather than just counts of categories which are often rather coarse. T-tests and Analysis of Variance (ANOVA) tests could then be used to check if the mean and variance of the simulated and survey data are statistically likely to be from the same population. However, the raw results of IPF are not conducive to such tests at the individual level because they do not contain whole individuals. Integerisation of the weight matrices is needed.

6.2 Integerisation

A question raised by this research is this: How do integerised IPF results compare with other (e.g. combinatorial optimisation) approaches to spatial microsimulation? Studies have compared non-integer results of IPF with alternative approaches (**?**), but not like-with-like.

6.3 Extensions to the basic model

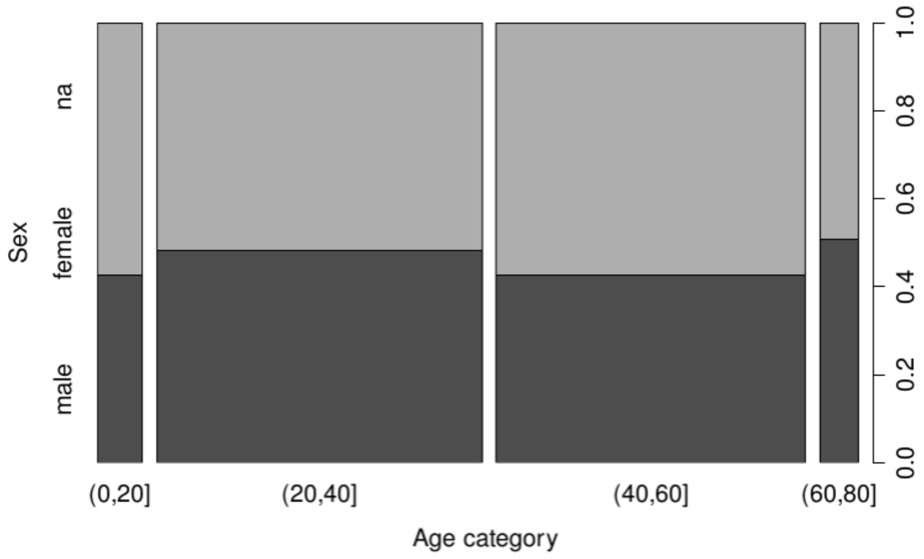


Figure 6.1: Diagnostic plot to check the sanity of age and sex inputs. (Square brackets indicate that the endpoint is not included in the set — see International Organization for Standardization (ISO) 80000-2:2009, formerly ISO 31-11 on "mathematical signs and symbols for use in physical sciences and technology").

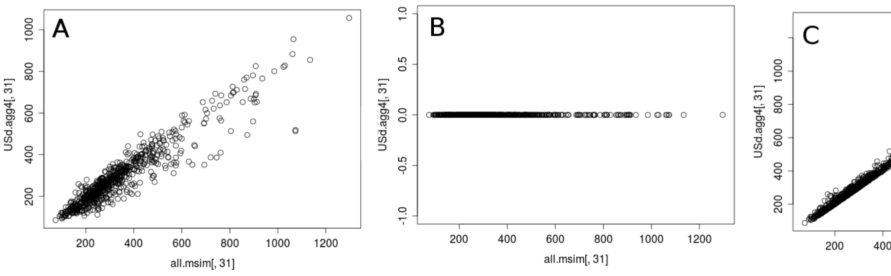


Figure 6.2: Three diagnostic plots used to identify a code error in the spatial microsimulation model (for the distance category 'travels 0–2 km to work'). The x-axis is census data, the y-axis is the simulated result. A) First plot analysed (for iteration 20); B) second plot, which illustrated the source of the problem, in the distance constraint; C) satisfactory diagnostic plot, after the problem had been resolved.

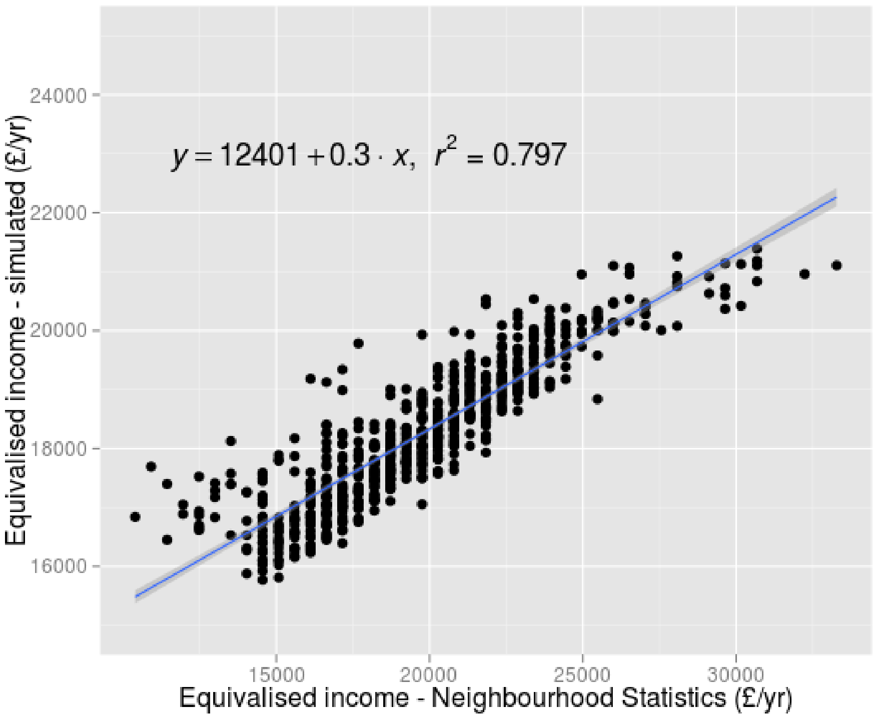
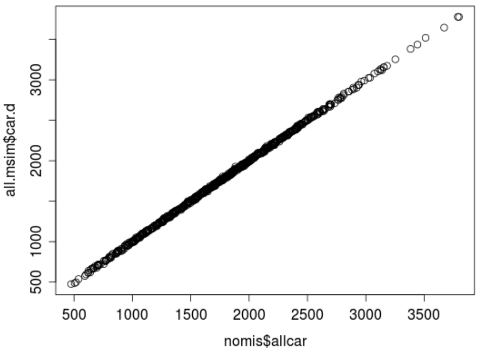


Figure 6.3: Scatter plot illustrating the correlation between mean income simulated from the model and official estimates at the MSOA leve.



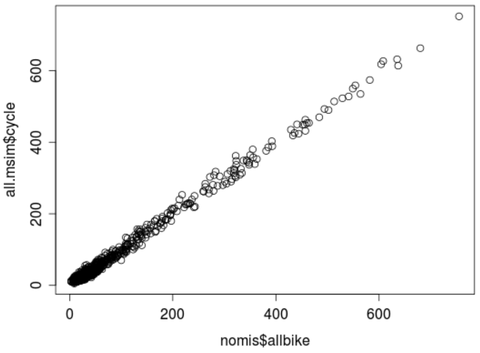
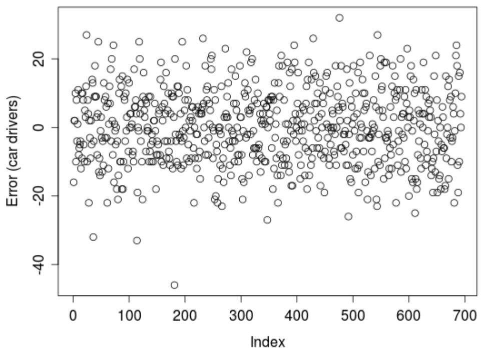


Figure 6.4: Scatter graphs illustrating the fit between Nomis and Casweb versions of the same census variables. The correlation (Pearson's r) is 0.9998 and 0.9969, for the number of car drivers and number of cyclists in each MSOA respectively.



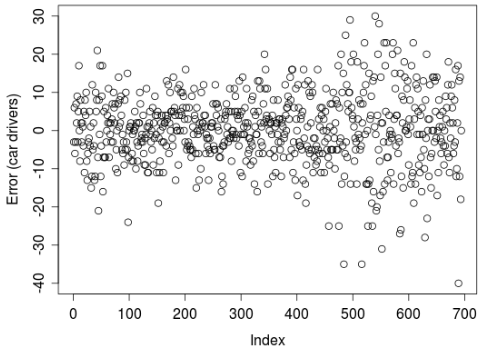


Figure 6.5: Errors (Casweb values – Nomis values) associated with car driver (right) and bicycle commuter (left) census variables.

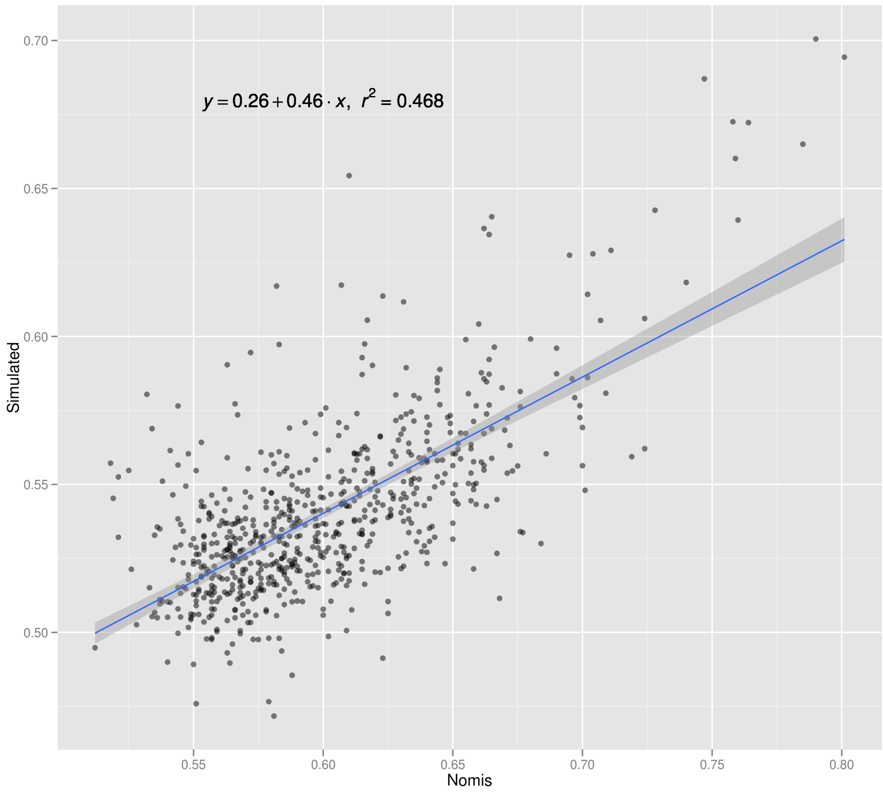


Figure 6.6: Scatter plot of the proportion of male drivers in each MSOA area in Yorkshire and the Humber according to simulated and Nomis data.

Chapter 7

Spatial microdata inputs into agent based models

Chapter 8

Conclusions and further resources

8.1 Acknowledgements

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