Advances in Population Synthesis: Fitting Many Attributes Per Agent and Fitting To Household and Person Margins Simultaneously

David R. Pritchard · Eric J. Miller

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Abstract Agent-based microsimulation models of transportation, land use or other socioeconomic processes require an initial synthetic population derived from census data, conventionally created using the Iterative Proportional Fitting (IPF) procedure. This paper introduces a novel computational method that allows the synthesis of many more attributes and finer attribute categories than previous approaches, both of which are long-standing limitations discussed in the literature. Additionally, a new approach is used to fit household and person zonal attribute distributions simultaneously. This technique was first adopted to address limitations specific to Canadian census data, but could also be useful in U.S. and other applications. The results of each new method are evaluated empirically in terms of goodness-of-fit.

Keywords iterative proportional fitting \cdot population synthesis \cdot microsimulation \cdot agent-based \cdot census microdata \cdot transportation models \cdot trip forecasting

1 Introduction

Agent-based microsimulation models forecast the future state of an aggregate system by simulating the behavior of a number of individual agents over time. These models are attracting interest from many fields, including activity-based travel demand modeling. The model output is usually the spatial arrangement of travel patterns (including the mode of travel used), and the agents are usually persons, families or households. The execution of such a model can be divided into two steps: the creation of an initial set of agents, their attributes and the system's state at some initial time; and a series of subsequent steps forward, where the state of each agent and the system as a whole is advanced by a timestep (for example, one year per step).

D.R. Pritchard Metrolinx, 20 Bay St. Suite 901 Toronto, ON, Canada M5S 1A4 E-mail: drpritch@gmail.com

E.J. Miller

Cities Centre, University of Toronto, 455 Spadina Ave., Suite 400, Toronto, ON, Canada M5S $2\mathrm{G8}$

The relationships between agents are also important. For example, members of a household do not act entirely independently; they share resources and may choose to travel together in a single vehicle, to adjust their travel patterns to suit each others' schedules, or to make decisions about home ownership based on all household members' needs. In an integrated land use/transportation model, major decisions such as household relocation are intimately linked to the behavior of persons in the household. Consequently, it is also important to have accurate relationships between agents and a realistic grouping of persons into households. The spatial distribution of attributes also needs to be accurate at both the household level and the person level.

Unfortunately, the census data often used to support microsimulation models does not make this possible. For privacy reasons, many national censuses remove spatial detail when providing detailed information about particular households or persons. In some countries, linkages between households and persons are also stripped. Consequently, "population synthesis" methods are necessary to fill in this information.

This paper focuses on three aspects of population synthesis. After an overview of previous work (Section 2), the conventional approach (Beckman et al 1996) is altered to support a larger number of attributes per agent (Section 3), adopting some ideas from an alternative reweighting approach (Williamson et al 1998). Second, a new approach to relationship synthesis is proposed that allows person- and household-level agents to be synthesized with the correct geographic distribution of attributes at both levels simultaneously (Section 4). The new relationship method is also applicable to datasets without linkages between the person and household levels, such as the Canadian census. Third, the implications of "random rounding" in the Canadian census are briefly discussed (Section 5). Finally, the effects of varying amounts of input data on the synthesis procedure are evaluated (Section 6) and concluding remarks (Sections 7 and 8).

While the methods were developed to support the ILUTE integrated land use/ transportation model (Salvini and Miller 2005), this paper is relevant to a broad group of socioeconomic models that use microsimulation methods.

1.1 Notation

A three-way contingency table \mathbf{n}_{ijk} (or sometimes \mathbf{n}) cross-classifies variables X, Y and Z into I, J and K categories respectively. Each cell n_{ijk} is a count of observations classified into category i of the first variable, category j of the second variable and category k of the third variable. The conventional notation \mathbf{n}_{i++} is used to indicate a one-way margin of \mathbf{n}_{ijk} . Each cell $n_{i++} = \sum_j \sum_k n_{ijk}$ of this margin contains the number of observations where variable X was observed in category i. The notation n is shorthand for n_{+++} , the total number of observations in table \mathbf{n}_{ijk} . Variable Z(k) will consistently represent geographic zones here.

2 Previous Work

2.1 Iterative Proportional Fitting

The IPF algorithm (Deming and Stephan 1940) is a method for adjusting a source contingency table (denoted with lower-case n) to match known marginal totals for some

target population (denoted with upper-case N). First, a "source" population is sampled and cross-classified to form a multiway table \mathbf{n}_{ij} . A similarly structured multiway table \mathbf{N}_{ij} is desired for some target population, but less information is available about the target: typically, some marginal totals \mathbf{N}_{i+} and \mathbf{N}_{+j} are known. The complete multiway table \mathbf{N}_{ij} of the target population is never known, but the IPF procedure is used to find an estimate $\hat{\mathbf{N}}_{ij}$. This is achieved through repeated modifications of the table \mathbf{n}_{ij} . The result is unique and exactly satisfies the margins, except in cases where entire rows/columns are zero in the source sample and non-zero in the margin. The method extends easily to higher dimensional tables cross-classifying more than two variables, and also to higher-dimension margins (Deming and Stephan 1940).

IPF minimizes discrimination information or relative entropy (Little and Wu 1991). That is, the fitted table $\hat{\mathbf{N}}$ minimizes

$$\sum_{i} \sum_{j} \hat{N}_{ij} \log(\hat{N}_{ij}/n_{ij}) \tag{1}$$

provided that zeroes are treated using the following convention (Csiszár 1975),

$$\log 0 = -\infty, \quad \log \frac{a}{0} = +\infty, \quad 0 \cdot \pm \infty = 0 \tag{2}$$

The relationship between a cell in a three-way fitted table and a non-zero cell in the source table can be expressed as

$$\log \hat{N}_{ijk} / n_{ijk} = \lambda + \lambda_{X(i)} + \lambda_{Y(j)} + \lambda_{Z(k)}$$
(3)

for \mathbf{N}_{i++} , \mathbf{N}_{+j+} and \mathbf{N}_{++k} margins, and some suitable choice of λ parameters (Stephan 1942; Agresti 2002). This has the exact same form as a log-linear model (Wickens 1989) and explains all of the variance of the data in the left-hand side. The number of parameters in the model is 1 + (I-1) + (J-1) + (K-1), proportional to the number of cells in the margins. A similar model can be constructed for any set of margins applied during the IPF procedure, by adding λ terms that correspond to the variables in the margins; the number of parameters remains proportional to the number of marginal cells. The presence of zeroes in the source table complicates the analysis, however.

The IPF procedure is capable of operating in the presence of zeroes in either the source table or the margins. A zero cell in the source table can be either a "sampling zero" where the sample—by chance—did not contain any observations for a particular cell. Alternatively, the zero could be a "structural zero" where the cell will be zero regardless of the sample chosen, typically when a particular combination of categories is impossibl. For example, the combination of "women aged 0–10" and "women with one child" would be a structural zero. Lacking any means of distinguishing sampling zeroes from structural zeroes, the IPF procedure will preserve zeroes from the source table in the fitted table.

2.2 Population Synthesis Using IPF

Census data is the primary source for agent-based transportation microsimulation models. Large-sample detailed cross-tabulations of one or two variables across many small geographic areas are the traditional form of census delivery, and are known as Summary Files in the U.S., Profile Tables or Basic Summary Tabulations (BSTs) in Canada, and Small Area Statistics in the U.K. In addition, a small sample of individual census records is commonly available. These samples consist of a list of individual persons (or families or households) drawn from some large geographic area, and are called Public-Use Microdata Samples (PUMS) or Files (PUMF) in the U.S. and Canada respectively, or a Sample of Anonymized Records in the U.K. The geographic area associated with a PUMS is the Public-Use Microdata Area (PUMA) in the U.S., and the Census Metropolitan Area (CMA) in Canada. In the U.S., each household in the PUMS is linked to specific individuals in the person PUMS. By contrast, the Canadian census omits these links for privacy reasons, and goes further to prevent overlap between the different PUMS samples; any person whose information is disclosed in the person PUMS is guaranteed to be excluded from the household PUMS. The Canadian census also provides some data aggregated to the household level and other data at the family level, whereas the U.S. census does not have a distinct family aggregation.

The standard procedures for using IPF in population synthesis with PUMS data were derived as part of the TRANSIMS project (Beckman et al 1996). Essentially, the PUMS data is used as the multiway source sample **n**, Summary Files are used to form the low-dimensional margins of **N** and the IPF procedure is used to adjust the source sample to fit the margins, resulting in a fitted table $\hat{\mathbf{N}}$. The original paper described two approaches for dealing with geography. In the zone-by-zone approach, one zone is fitted at a time using the margins of **N** for that zone alone. This assumes that every zone shares the correlation structure of the PUMA defined in **n**. The multizone approach takes the opposite tack: all zones are fitted simultaneously by adding a new dimension to the marginal table **N** for the zone code. The details are a little convoluted, but Figure 1 provides a succinct explanation.

The IPF process produces a multiway contingency table for the zones, where each cell contains a real-valued count $\hat{N}_{ij\kappa}$ of the number of agents with a particular set of attributes X = i and Y = j in zone $Z = \kappa$. However, to define a discrete set of agents integer counts are required. Deterministic rounding of the counts is not a satisfactory "integerization" procedure for three reasons: the rounded table may not be the best solution in terms of discrimination information; the rounded table may not offer as good a fit to margins as other integerization procedures; and rounding may bias the estimates, particularly for cells representing "rare" characteristics with a count under 0.5. The original paper handled this problem by treating the fitted table as a joint probability mass function (PMF), and then used N Monte Carlo draws from this PMF to select N individual cells (Beckman et al 1996). These draws can be tabulated to give an integerized approximation $\hat{\mathbf{N}}'$ of $\hat{\mathbf{N}}$. This is an effective way to avoid biasing problems, but at the expense of introducing a nondeterministic step into the synthesis.

There are several documented applications of the IPF method for population synthesis (Bowman 2004).

2.3 Reweighting and Combinatorial Optimization

The primary alternative to the Iterative Proportional Fitting algorithm is the reweighting approach (Williamson et al 1998), also sometimes known as combinatorial optimization. Williamson et al proposed a zone-by-zone method with a different parameterization of the problem: instead of using a contingency table of real-valued counts, they chose a list representation with one row per PUMS entry, each with an integer



Fig. 1 An illustration of the multizone fitting procedure (Beckman et al 1996). In the left half, Z is ignored and the PUMS is adjusted to match the summary tables; they differ because the PUMS is derived from a smaller sample than the summary tables. In the right half, the variable Z(k) is added to represent the K zones that make up the PUMA. A constant initial table filled with ones is used for a second IPF, which is fitted to the summary tables and the adjusted PUMS. The summary tables now show variation of X by zone Z (and likewise $Y \times Z$), while the adjusted PUMS provides information about the association between X and Y.

weight. Within a single zone, they used weights of either zero or one on each PUMS row, allowing no replication of PUMS observations within a single zone.

To estimate the weights, they used various optimization procedures to find the set of $\{0, 1\}$ weights yielding the best fit to the Summary Tables for a single zone. They considered several different measures of fit, and compared different optimization procedures including hill-climbing, simulated annealing and genetic algorithms. By solving directly for integer weights, a better fit to the Summary Tables might be obtained than with IPF methods where Monte Carlo integerization step harms the fit.

The reweighting approach has three primary weaknesses. First, the attribute association observed in the PUMS (\mathbf{n}_{ij}) is not preserved by the algorithm. The IPF method has an explicit formula defining the relationship between the fitted table $\hat{\mathbf{N}}_{ij}$ and the PUMS table \mathbf{n}_{ij} in equation (3). Beckman et al.'s multizone approach also treats the PUMS association pattern for the entire PUMA as a constraint, and ensures that the full population matches that association pattern. The reweighting method does operate on the PUMS, and an initial random choice of weights will roughly match the association pattern of the PUMS. However, the reweighting procedure does not make any effort to preserve that association pattern.

Secondly, the reweighting method is very computationally expensive. When solving for a single zone κ , there are $n \{0, 1\}$ weights, one for each PUMS entry. However, this gives rise to $\binom{n}{N_{++\kappa}}$ possible combinations; Williamson et al (1998) called it "incredibly large." Of course, the optimization procedures are intelligent enough to explore this

space selectively and avoid an exhaustive search; nevertheless, Huang and Williamson (2001) reported a runtime of 33 hours using an 800MHz processor.

Finally, the reweighting method uses $n \times K$ weights to represent a K-zone area. This parameter space is quite large; larger, in fact, than the population itself. It is not surprising that good fits can be achieved with a large number of parameters, but the method is not particularly parsimonious and may overfit the Summary Tables. It is likely that a simpler model with fewer parameters could achieve as good a fit, and would generalize better from the small (2–5%) PUMS sample to the full population.

3 Sparse List-Based Data Structure

For a microsimulation model spanning many aspects of society and the economy it is useful to be able to associate a range of attributes with each agent. Different attributes are useful for different aspects of the agent's behavior. For a person agent, labor force activity, occupation, industry and income attributes are useful for understanding his/ her participation in the labor force. Meanwhile, age, marital status, gender and education attributes might be useful for predicting demographics.

However, as more attributes are associated with an agent, the number of cells in the corresponding multiway contingency table grows exponentially. A multiway contingency table representing the association pattern between attributes has $I \times J \times K \times \ldots$ cells. If a new attribute with L categories is added, then L times more cells are needed. Asymptotically, the storage space is exponential in the number of attributes. As a result, fitting more than eight attributes with a multizone IPF procedure typically requires more memory than available on a desktop computer. However, the table itself is cross-classifying a fixed number of observations (i.e., a PUMS), and is extremely sparse when a large number of attributes are included. Is there a way to exploit this sparsity and synthesize a large number of attributes?

Sparsity is a familiar problem in numerical methods. Many branches of science store large sparse 2D matrices using special data structures that hold only the nonzero sections of the matrix, instead of using a complete array that includes cells for every zero. The IPF method itself has little impact on the sparsity pattern of a table, and does not require a complete representation of the table. After the first iteration of fits to the constraints, the final sparsity pattern is essentially known; some cells may eventually converge to near-zero values, but few other changes occur.

The benefits of using a sparse data structure are substantial: efficient use of computer memory, flexibility of aggregation and easier linking of data sources (Williamson et al 1998). In terms of efficiency, the method described here allows the IPF algorithm to be implemented using storage proportional to the number of non-zero cells in the initial table. For agent synthesis with the zone-by-zone method, this is proportional to n (the number of observations in the PUMS) multiplied by d (the number of attributes to fit). The multizone method combines several IPF stages, and requires considerably more memory: a similar O(nd) in the first stage, but O(n(d+K)) in the second stage (expressed in order of magnitude terms using the "Big O" Landau notation commonly used in computer science).

It is helpful to consider a real example: synthesis of family agents using the 1986 Family PUMS for the Toronto CMA, which contains 9061 families. (This paper uses 1986 data only because it is the base year for the ILUTE land use/transportation model; this base year allows model validation over the 1986–2006 simulation period.)

(a)										
			Co-ord	linates						
	Index	FSTRUC	Rooms Tenure			NCHILD	Weight			
-	1	Husband-wife	7	Owned		3	8	81.8 70.9		
	2	Lone female parent	4	Rented		0	7			
	3	Husband-wife	9	Rented		0		54.8		
	4	Husband-wife	9	Owned		0	86.2			
	9060	Husband-wife	9	Rented		0	64.8			
_	9061	Husband-wife	6	Rented		0	10	00.3		
(b)										
		Co-ordin	ates		Weight					
	Index	FSTRUC		NCHILD	Zone1	Zone2		Zone731		
	1	Husband-wife		3	0.000	0.121		0.021		
	2	Lone female parent		0	0.000	0.212		0.020		
	3	Husband-wife		0	0.000	0.244		0.143		
	4	Husband-wife		0	0.002	0.037		0.019		
	9060	Husband-wife		0	0.000	0.349		0.011		
	9061	Husband-wife		0	0.004	0.213		0.074		

Fig. 2 Format of a sparse list-based data structure for Iterative Proportional Fitting As shown, each row corresponds to a PUMS entry. The columns give the co-ordinates of each PUMS entry within the high-dimensional array. Each row also stores (a) a single weight when synthesizing only attributes present in the PUMS (e.g., an IPF without geography, such as IPF for a single zone in the zone-by-zone method); or (b) a set of weights, corresponding to the categories of an attribute absent from the PUMS (e.g., a multizone IPF where the zone attribute is not present in the PUMS).

For synthesis of 10 attributes using a zone-by-zone method, the complete representation requires 52.5 MB of storage while a sparse scheme needs only 0.1 MB. When a multizone method is used for the 731 zones, complete storage would require a prohibitive 38 369 MB while sparse storage needs only 27 MB. For small numbers of attributes, however, the complete representation is more efficient.

There are many types of data structures that could be used to represent a sparse high dimensional contingency table. The data structure proposed here is not the most efficient, but is conceptually simple. It borrows directly from the reweighting/ combinatorial optimization method (Williamson et al 1998): the data is represented as a list of the PUMS microdata entries, with a weight attached to each. The weight is an expansion factor, representing the number of times to replicate that record to form a complete population. While the representation used by the combinatorial optimization method includes only integer weights and operates on a zone-by-zone basis, the approach used here behaves exactly like IPF and hence allows fractional weights. With a small extension, it can also support multiple zones: instead of attaching one weight to each PUMS entry, K weights are used. An illustration of the data structure is shown in Figure 2.

Flexible aggregation is a real advantage of a list-based representation (Williamson et al 1998). Complete array storage is proportional to the number of categories used for each attributes, while the sparse storage scheme is not affected by the categorization of the attributes. Many applications of IPF that used complete arrays were forced to abandon detailed categorization schemes to conserve space and allow more attributes to be synthesized (see for example Arentze and Timmermans 2005; Auld et al 2009). This in turn makes it difficult to apply several margins, since different margins may categorize a single attribute differently. When a large number of categories are possible,

however, the attribute can be represented with a fine categorization and collapsed onthe-fly to different coarse categorizations as required during the fitting procedure.

3.1 Algorithmic Details

To implement the IPF algorithm with a sparse list structure, the following operations are necessary:

- Set the initial weights.
- Convert and collapse list to a table with the dimensions of a target margin. For example, collapse to $\hat{\mathbf{N}}_{i+}$ in preparation for applying margin \mathbf{N}_{i+} .
- For each cell in the collapsed table, update the list entries that contributed to that cell. For example, for cell N_{i+} , the contributing cells are all rows in the list where X = i.

Since the target population margins remain stored as complete arrays, these operations are relatively straightforward. The collapse operation can be done in a single pass over the list, using the category numbers in each list row as co-ordinates into the complete array that stores the collapsed table. The update operation can likewise be done in a single pass over the list. Both operations are fast with complexity equal to the storage cost, $\mathcal{O}(nd)$.

Setting the initial weights requires a little more work and is slightly counterintuitive. With a complete array representation, the initial table is set to the PUMS cross-tabulation for a zone-by-zone synthesis and set to a uniform distribution (1.0 in all cells) for multizone synthesis. In the sparse representation used here, this changes slightly since there is one weight per PUMS entry instead of groups of PUMS entries in each cell. Consequently, the initial row weights need to be set to 1.0 for the zone-by-zone method. For the multizone method, the sum of the weights in the r rows that contribute to a single cell in the equivalent complete table needs to add to one, and the individual weights are therefore 1/r. To allow easy calculation of r, the list needs to be sorted by the table dimension co-ordinates, grouping the rows that contribute to a single cell. Thus the initial weights can be set in $\mathcal{O}(n \log n)$ time.

Additionally, the multizone IPF procedure requires a fit to the distribution of all non-geographic variables simultaneously. (See the $\hat{\mathbf{N}}_{ij+}$ margin on the right half of Figure 1.) This margin is high-dimensional—it includes all variables except for the geographic variable—but is also stored as a sparse list with a single weight per row. This weight can be treated as a constraint on the total for the weights in each row, and suitable collapse/update procedures are then easily defined. The computation cost is still $\mathcal{O}(n(d+K))$ for this type of constraint.

Finally, integerization for this sparse structure is little changed. The list of weights (or 2D array of weights for multizone) is normalized and treated as a PMF and individual entries are synthesized using Monte Carlo draws.

3.2 Discussion

This sparse data structure removes a substantial limitation from the IPF algorithm, but also raises new questions. Is there a limit to the number of attributes that can be synthesized? If there is a limit, how is it related to the size n of the PUMS sample?

The answers to these questions remain elusive. The issue likely hinges on the statistical validity of high-dimensional contingency tables. These tables are inherently sparse, with a large fraction of the non-empty cells containing only one observation and the number of cells is often much larger than the number of observations. In other words, the sample does not provide a statistically meaningful estimate of the probability distribution for such a high dimensional table. However, the high-dimensional table can be collapsed to produce 2D or 3D tables, each of which is adequately sampled and gives a statistically valid distribution of counts. For example, in an 8-way crossclassification of a 1986 Toronto census PUMS containing 9061 families, 99.7% of the 984 150 cells were zero. However, one of the table's three-way margins had 54 cells and a median of 30 observations per cell. There are $\binom{8}{3} = 56$ possible choices of variables to form a 3-way margin of the 8-way table, and the observations per cell in each margin is comparable. Consequently, while a sparse 8-way table does not provide statistically meaningful information about 8-variable interaction, it could be viewed as a means of linking the many 2- or 3-way tables formed by its margins.

4 Synthesizing Agent Relationships

In this section, the discussion shifts from a single agent type (e.g., family agents) to the synthesis of multiple agent types simultaneously: for example, person agents and household agents.

In the U.S. context, the relationship between these types of agents can be observed directly in the PUMS data. Synthesis of both types of agents typically uses a top-down approach, where households are created with IPF (fitting only against household-level attributes) and subsequently the links built into the U.S. PUMS are used to synthesize the individual persons within the households (Beckman et al 1996; Barrett et al 2003). The synthesized persons are naturally grouped into plausible households, because the procedure draws from observed groupings of persons in the PUMS.

By contrast, this approach is impossible in the Canadian census, where the PUMS for households contains only limited information on the persons within the household, and no way of linking to the detailed census data on individual persons. While Canadian data limitations were the original motivation for developing a new method, other benefits became apparent after the method was developed. For non-Canadian applications, the method offers two key advantages over the conventional approach to synthesizing households:

- can achieve a good fit for both household and person attributes simultaneously, at the level of individual zones;
- produces greater variation in the composition of households. While PUMS households are replicated as in the conventional approach, each replicate of a PUMS household typically contains a different set of person agents.

Several previous papers have attempted to deal with the issue of fitting against both household and person attributes. Guo and Bhat (2007) built on the conventional approach, retaining the U.S. census' linkage between households and persons, but modifying the Monte Carlo synthesis stage to attempt a fit at both the household level and the person level simultaneously. Only a few person-level attributes were incorporated: gender and age. The constraints were somewhat loose and *ad hoc*, since the procedure Ye et al (2009) tackled the same problem of person-level attributes. They applied IPF twice independently, first on the household level and second on the person level, obtaining two separate sets of weights. A heuristic procedure was then used to solve for household-level weights that could simultaneously satisfy both IPF-derived sets of weights. The method showed good results in a case study with three attributes at both the household and person levels, but the authors acknowledged that both the total number of attributes and the number of categories per attribute play an important role in the performance of the algorithm. It is likely that the method would have difficulty with the large number of attributes and categories contemplated in this paper.

Arentze and Timmermans (2005) only synthesized for the top-level agent, the household. Their synthesis included the age and labor force activity of both husband and wife, and the number of children in the household. They did not connect this to a separate synthesis of persons with detailed individual attributes, but by synthesizing at an aggregate level they guaranteed that the population was consistent and satisfied key constraints between family members, in the same manner as Beckman et al (1996).

Guan (2002) used a bottom-up approach to build families using the Canadian census. The person agents were synthesized first, and then assembled to form families. Children were grouped together (and constrained to have similar ages), then attached to parents. Constraints between parent/child ages and husband/wife ages were included, although there are some drawbacks to the method used for enforcement. Guan likewise used a bottom-up approach to combine families and non-family persons into households.

4.1 Grouping persons

Any method for synthesizing relationships between persons must produce credible groupings of persons (into families and/or households). Suppose that a population of person agents has been synthesized, with a limited amount of information about their relationships in families (such as an attribute FSTRUC, which classifies a person as married, a lone parent, a child living with parent(s), or a non-family person). In the absence of any information about how families form, the persons could be formed into families in a naïve manner: randomly select male married persons and attach them to female married persons, and randomly attach children to couples or lone parents. Immediately, problems would emerge: some persons would be associated in implausible manners, such as marriages with age differences over 50 years, marriages between persons living at opposite ends of the city, or parents who are younger than their children.

A well-designed relationship synthesis procedure should carefully avoid such problems. A good choice of relationships satisfies certain *constraints* between agents' attributes, such as the mother being older than her child, or the married couple living in the same zone. It also follows known *probability distributions*, so that marriages with age differences over 50 years have a low but non-zero incidence.

Most constraints and probability distributions are observed in microdata samples of aggregate agents such as families or households. A complete Family PUMS in the Canadian census includes the ages of mothers and children, and none of the records includes a mother who is younger than her children. Similarly, only a small fraction of the records include marriages between couples with ages differing by more than 50 years. The question, however, is one of method: how can relationships between agents be formed to ensure that the desired constraints are satisfied?

As Guo and Bhat (2007), Ye et al (2009) and Guan (2002) found, working at the household/family and person levels simultaneously can introduce conflicts between the competing goals of achieving good fit at both levels. The family population may contain 50 husband-wife families in zone k where the husband has age i, while the person population contains only 46 married males of age i in zone k. In the face of such inconsistencies, either families or persons must be changed: a family could be attached to a male of age $i' \neq i$, or a person could be modified to fit the family. In both cases, either the family or person population is deemed "incorrect" and modified. The editing procedures are difficult to perform, and inherently *ad hoc*. Furthermore, as the number of overlapping attributes between the two populations grows, inconsistencies become quite prevalent.

What are the sources of these inconsistencies? They come from two places: first, the fitting procedure used to estimate the population distribution $\hat{\mathbf{N}}^P$ for persons and $\hat{\mathbf{N}}^F$ for families may not give the same totals for a given set of common attributes. Second, even if $\hat{\mathbf{N}}^P$ and $\hat{\mathbf{N}}^F$ could be made to agree on all shared attributes, the populations produced by independent Monte Carlo synthesis on the two tables (used by Guan) may not agree, since the Monte Carlo procedure is non-deterministic. In the following sections, a method is proposed to resolve these two issues.

4.2 Fitting Populations Together

For the purposes of discussion, consider a simple synthesis example: synthesizing husband-wife families. Suppose that the universe of persons includes all persons, with attributes for gender SEXP(g), family status FSTRUC(h), age AGEP(i), education EDUP(j) and zone ZONE(k). The universe of families includes only husband-wife couples, with attributes for the age of husband AGEM(i_m) and wife AGEF(i_f), and zone ZONE(k). IPF has already been used to estimate the contingency table cross-classifying persons ($\hat{\mathbf{N}}_{ghijk}^P$) and likewise for the table of families ($\hat{\mathbf{N}}_{i_m i_f k}^F$). The shared attributes between the two populations are age and zone, and implicitly gender. The two universes do not overlap directly, since only a fraction of the persons belong to husband-wife families; the others may be lone parents, children, or non-family persons, and are categorized as such using the FSTRUC attribute.

In order for consistency between $\hat{\mathbf{N}}^P$ and $\hat{\mathbf{N}}^F$, the following must be met for h = husband-wife and any choice of i, k:

$$\hat{N}_{ghi+k}^{P} = \begin{cases} \hat{N}_{i+k}^{F} & \text{for } g=male\\ \hat{N}_{+ik}^{F} & \text{for } g=female \end{cases}$$
(4)

That is, the number of married males of age i in zone k must be the same as the number of husband-wife families with husband of age i in zone k. While this might appear simple, it is often not possible with the available data. A margin \mathbf{N}_{g+i+k}^{P} giving the SEXP × AGEP × ZONE distribution is probably available to apply to the person population. However, a similar margin for just *married* males is not likely to exist for the family population; instead, the age breakdown for married males in the family usually comes from the PUMS alone. As a result, equation (4) is not satisfied.

One suggestion immediately leaps to mind: if the person population is fitted with IPF first and $\hat{\mathbf{N}}^P$ is known, the slice of \hat{N}^P_{ghi+k} where g = male and h = husband-wife could be applied as a margin to the family fitting procedure, and likewise for g = female. This is entirely feasible, and does indeed guarantee matching totals between the populations. The approach can be used for the full set of attributes shared between the individual and family populations. There is one downside, however: it can only be performed in one direction. The family table can be fitted to the person table or vice versa, but they cannot be fitted simultaneously.

Finally, there remains one wrinkle: it is possible that the family population will still not be able to fit the total margin from the individual population, due to a different sparsity pattern. For example, if the family PUMS includes no families where the male is 15–19 years old but the individual PUMS does include a married male of that age, then the fit cannot be achieved. This is rarely an issue when a small number of attributes are shared, but when a large number of attributes are shared between the two populations it is readily observed. The simplest solution is to minimize the number of shared attributes, or to use a coarse categorization for the purposes of linking the two sets of attributes.

Alternatively, the two PUMS could be cross-classified using the shared attributes and forced to agree. For example, for g = male and h = husband-wife, then the pattern of zeros in \mathbf{n}_{ghi++}^{P} and \mathbf{n}_{i++}^{F} could be forced to agree by setting cells to zero in one or both tables. (In the earlier example, this would remove the married male of age 15– 19 from the Person PUMS.) The person population is then fitted using this modified PUMS, and the family population is then fitted to the margin of the person population.

4.3 Conditioned Monte Carlo

The second problem with IPF-based synthesis stems from the independent Monte Carlo draws used to synthesize persons and families. For example, suppose that mutually fitted tables $\hat{\mathbf{N}}^{P}$ and $\hat{\mathbf{N}}^{F}$ are used with Monte Carlo to produce a complete population of persons and families $\hat{\mathbf{N}'}^{P}$ and $\hat{\mathbf{N}'}^{F}$. If it can be guaranteed for g = male and h = husband-wife that

$$\hat{\mathbf{N}'}_{ghi+k}^{P} = \hat{\mathbf{N}'}_{i+k}^{F} \tag{5}$$

(and likewise for g = female), then a perfectly consistent set of connections between persons and families is possible. How can equation (5) be satisfied?

A simplistic solution would be a stratified sampling scheme: for each combination of *i* and *k*, select a number of individuals to synthesize and make exactly that many draws from the subtables $\hat{\mathbf{N}}_{++i+k}^{P}$ and $\hat{\mathbf{N}}_{i+k}^{F}$. This approach breaks down when the number of strata grows large, as it inevitably does when more than one attribute is shared between persons and families.

The problem becomes clearer once the reason for mismatches is recognized. Suppose a Monte Carlo draw selects a family with husband age i in zone k. This random draw is not synchronized with the draws from the person population, requiring a person of age iin zone k to be drawn; the two draws are independent. Instead, synchronization could be achieved by *conditioning* the person population draws on the family population draws. Instead of selecting a random value from the joint distribution

P(SEXP, FSTRUC, AGEP, EDUP, ZONE)

of the person population, a draw from the conditional distribution

P(EDUP | SEXP = male, FSTRUC = husband-wife, AGEP = i, ZONE = k)

could be used, and a similar draw for the wife. Converting the joint distribution generated by IPF to a conditional distribution is an extremely easy operation.

This reversal of the problem guarantees that equation (5) is satisfied, and allows consistent relationships to be built between agents. While it has been described here in a top-down manner (from family to person), it can be applied in either direction.

4.4 Discussion

As demonstrated, it is possible to synthesize persons and relate them together to form families, while still guaranteeing that the resulting populations of persons and families approximately satisfy the fitted tables $\hat{\mathbf{N}}^P$ and $\hat{\mathbf{N}}^F$. By carefully choosing a set of shared attributes between the person and family agents and using conditional synthesis, a limited number of constraints can be applied to the relationship formation process. In the example discussed earlier, the ages of husband/wife were constrained; in a more realistic example, the labor force activity of husband/wife, the number of children and the ages of children might also be constrained. Furthermore, multiple levels of agent aggregation could be defined: families and persons could be further grouped into households and attached to dwelling units.

The synthesis order for the different levels of aggregation can be varied as required, using either a top-down or bottom-up approach. However, the method is still limited in the types of relationships it can synthesize: it can only represent nesting relationships. Each individual person can only belong to one family, which belongs to one household. Other types of relationships cannot be synthesized using this method, such as a person's membership in another group (e.g., a job with an employer).

While this method is clearly useful for Canadian data that lacks links between the household and person level, is it useful in other contexts? The answer depends on whether the benefits (simultaneous attribute fitting at the household and person level, and greater variation in household composition) outweigh the costs (implementation difficulty, and the synthetic nature of the household/person relationships).

5 Fitting to Randomly Rounded Margins

Many census agencies apply random rounding procedures to published tables, including the agencies in Canada, the United Kingdom and New Zealand. Each agency has a base b that it uses, and then modifies a cell count N_{i+} by rounded up to the nearest multiple of b with a probability p, or down with a probability 1 - p. In most applications, a procedure called *unbiased* random rounding is used, where $p = (N_{i+} \mod b)/b$. The alternative is called *unrestricted* random rounding, where p is constant and independent of the cell values; for example, with p = 0.5 it is equally likely that a cell will be rounded up or down.

For example, cells and marginal totals in Canadian census tables are randomly rounded up or down to a multiple of b = 5 using the unbiased procedure. For a cell with a count of $N_{i+} = 34$, there is a 20% probability that it is published as $\tilde{N}_{i+} = 30$ and an 80% probability that it is published as $\tilde{N}_{i+} = 35$. Most importantly, the expected value is equal to that of the unrounded count; it is therefore an unbiased random rounding procedure.

This can lead to conflicts between tables (Huang and Williamson 2001): two different cross-tabulations of the same variable or set of variables may be randomly rounded to different values (for example, the X margin of the $X \times Y$ and $X \times Z$ tables). The standard IPF procedure will not converge in this situation. The procedure is also unable to take into account the fact that margins do not need to be fitted exactly, since there is a reasonable chance that the correct count is within ± 4 of the reported count.

Two approaches were used in this work to deal with random rounding in the Canadian census data: a modification to the IPF termination criterion, and the use of hierarchical marginal tables.

5.1 Hierarchical Margins

For each cross-tabulation, statistical agencies publish a hierarchy of margins, and these margins are rounded independently of the cells in the table. For a three-way table N_{ijk} randomly rounded to give \tilde{N}_{ijk} , the data release will also include randomly rounded two-way margins \tilde{N}_{ij+} , \tilde{N}_{i+k} and \tilde{N}_{+jk} , one-way margins \tilde{N}_{i++} , \tilde{N}_{+j+} and \tilde{N}_{++k} , and a zero-way total \tilde{N}_{+++} . The sum of the cells does not necessarily match the marginal total. For example, the sum $\sum_k \tilde{N}_{ijk}$ includes K randomly rounded counts. The expected value of this sum is the true count N_{ij+} , but the variance is large and the sum could be off by as much as K(b-1) in the worst case. By contrast, the reported marginal total \tilde{N}_{ij+} also has the correct expected value, but its error is at most b-1.

For this reason, it seems sensible to include the hierarchical margins in the fitting procedure, in addition to the detailed cross-tabulation itself.

6 Evaluation

It is challenging to evaluate the results of a data synthesis procedure. If any form of complete "ground truth" were known, the synthetic population could be tested for goodness-of-fit against the true population's characteristics; instead only partial views of truth are available in smaller, four-way tables.

In theory, IPF-based procedures have many of the qualities necessary for a good synthesis: an exact fit to their margins, while minimizing the changes to the PUMS (using the discrimination information criterion). This does not mean that the full synthesis procedure is ideal: the fit will almost certainly be poorer after Monte Carlo (or conditional Monte Carlo). Furthermore, it still leaves a major question open: how much data is sufficient for a "good" synthesis? Are the PUMS and multidimensional margins both necessary, or could a good population be constructed with one of these two types of data? Does the multizone method offer a significant improvement over the zone-by-zone approach?

To investigate these questions, a series of experiments was conducted. The source data was from the 1986 census for the Toronto CMA, which is a single PUMA in the Canadian system. The synthetic population is a set of person agents with eight attributes each, described in Pritchard (2008). In the absence of ground truth, the synthetic population is evaluated in terms of its goodness-of-fit to a large collection of low-dimensional contingency tables. These validation tables are divided into the following groups:

- 1. One-dimensional margins for the entire PUMA, for each attribute.
- 2. One-dimensional margins by zone for each attribute.
- 3. Higher-dimensional Summary Tables for the entire PUMA.
- 4. Higher-dimensional Summary Tables by zone.
- 5. Higher-dimensional margins from PUMS that are unavailable in summary tables. A selection of 2D and 3D margins are taken from the PUMS after fitting each to the 1–3D margins in the Summary Tables.

After cross-classifying the synthetic population to form one table $\hat{\mathbf{N}}_{ijk}$, it can be compared to a validation table \mathbf{N}_{ijk} using a goodness-of-fit statistic. While there are sound theoretical reasons to prefer information-based statistics like Minimum Discrimination Information (equivalent to the G^2 statistic in log-linear models), distance-based metrics are more common in the literature. The Standardized Root Mean Square Error (SRMSE) statistic was chosen as a good distance-based metric for measuring matrix goodness-of-fit (Knudsen and Fotheringham 1986). Its formula is given by

$$SRMSE = \frac{\sqrt{\frac{1}{IJK} \sum_{i,j,k} (\hat{N}_{ijk} - N_{ijk})^2}}{\frac{1}{IJK} \sum_{i,j,k} N_{ijk}}$$
(6)

Like any distance-based statistic, a value of zero indicates a perfect fit. The RMS statistic (numerator) is standardized by the average cell value (denominator), in order for the statistic to be comparable for tables of different sizes. The upper limit of the SRMSE statistic is variable but is often assumed to be 1.0 (Knudsen and Fotheringham 1986).

This statistic is calculated for each of the validation tables in turn and the goodnessof-fit statistics in each group are then averaged together to give an overall goodnessof-fit for the group.

6.1 Tests of IPF Method and Input Margins

In the first series of experiments, the IPF procedure is tested with different inputs to see how the quality of fit is affected. Three questions are tested simultaneously using a set of ten fits, labeled I1 through I10. The input data included in each experiment are shown together with the output goodness-of-fit in Table 1. I6 represents a "typical" application of IPF for population synthesis: a zone-by-zone approach using 1D margins.

- Source Sample: How does the initial table in IPF affect the result? Can a good fit be obtained with a constant initial table (I1, I3, I5, I7), or is the PUMS necessary (I2, I4, I6, I8)? The results show an order of magnitude better fit with the PUMS. Note however the results for I6 in validation group 4: there are geographic variations in the 2–3D association pattern that are not explained by the combination of the PUMS and 1D margins with geography.

- 1D Margins: Are 1D margins sufficient (I1, I2, I5, I6, I9), or does a better fit result when 2D and 3D margins are applied (I3, I4, I7, I8, I10)? While the information in validation group 3 can be captured fairly well by the PUMS (albeit with a smaller sample size), the real benefit of 2D and 3D margins shows up in validation group 4, where a good fit is only achieved in I7, I8 and I10.
- Geography: What is the difference between the zone-by-zone (I5–I8) and multizone approach (I9–I10) to geographic variation? (The geography-free approach is provided for contrast in I1–I4.) As reported by others (Beckman et al 1996), the difference in fit is not large. The main difference can be seen in validation group 5: the multizone approach treats the PUMS as a constraint with equal importance to the marginal constraints, and achieves a better fit against 2D and 3D attributes that are not covered by the marginal tables. While the results are clearly better for the multizone approach, it does require additional computational resources.

6.2 Effects of Monte Carlo

The second series of experiments tests the effects of both the conventional Monte Carlo integerization procedure and the conditional Monte Carlo for relationships.

	Inputs						Me	thod				Output				
Margins				_						$\frac{\text{SRMSE} \times 1000 \text{ by table,}}{\text{grouped and averaged}}$						
Experiment	1. 1D STs (entire PUMA)	2. 1D STs (by zone)	3. 2–3D STs (entire PUMA)	4. $2-3D$ STs (by zone)	5. PUMS	Source sample	Geography (# zones at a time)	Monte Carlo	Conditioned Monte Carlo		1. 1D STs (entire PUMA)	2. 1D STs (by zone)	3. 2–3D STs (entire PUMA)	4. 2–3D STs (by zone)	5. 2–3D (only in PUMS)	
I1 I0	1					1	none			-	1	285	192	566	883	
12	1					PUMS	none				1	285	15	522	38 795	
15 14	· /		· /			DIMS	none				1	200	2	522	135	
14 I5	v	1	v			1 0 101	one				4	200	187^{2}	$\frac{522}{252}$	849	
I6		1				PUMS	one				1	3	19	130	73	
17		1		1		1	one				2	2	7	3	659	
I8		1		1		PUMS	one				1	1	3	3	56	
I9	1	1			\checkmark^a	1	multi				0	3	15	131	38	
I10	1	1	1	1	\checkmark^{b}	1	multi				0	1	0	3	0	
M0	1	1	1	1	\checkmark^{b}	1	multi			-	0	1	0	3	0	
M1	1	1	1	1	\checkmark^{b}	1	multi	1			3	39	3	80	12	
M2	1	1	1	1	\checkmark^{b}	1	multi		✓		8	58	7	99	21	

Table 1 Effects of Input Data and Conditioned Monte Carlo on Synthesis.

 a PUMS fitted to 1D margins

^b PUMS fitted to 2–3D margins

Table 2 Input margins applied to household, person and family levels during population synthesis (in addition to the all-way interaction derived from the PUMS, excluding zone). The final population achieves a good fit to all tables simultaneously.

Household					
Zone × Dwelling type × Tenure Zone × Dwelling type × Num. persons Zone × Dwelling type × Dwelling age Zone × Dwelling type × Num. rooms Zone × Dwelling payments × Num. families × Tenure Zone × Num. families × Num. persons					
Family					
Zone × Family structure × Num. children Zone × Num. children aged $0-5 \times 6-14 \times 15-17 \times 18-24 \times 25-$ Zone × Num. children aged $0-5 \times 6+ \times$ Labor activity (female)					
Person					
$\begin{array}{l} \text{Zone} \times \text{Sex} \times \text{Income} \\ \text{Zone} \times \text{Sex} \times \text{Age} \times \text{Family status} \\ \text{Zone} \times \text{Sex} \times \text{Age} \times \text{Labor activity} \\ \text{Zone} \times \text{Sex} \times \text{Age} \times \text{Education} \\ \text{Zone} \times \text{Sex} \times \text{Education} \times \text{Labor activity} \\ \text{Zone} \times \text{Sex} \times \text{Occupation} \end{array}$					

The design and results of these experiments are also in Table 1 under labels M0–M2. Because the Monte Carlo procedure is non-deterministic, the reported SRMSE is an average over 30 trials. The first experiment M0 is the null case: IPF before Monte Carlo. Experiment M1 shows the conventional Monte Carlo procedure, where a set of persons are synthesized directly from the IPF-fitted table for persons. Experiment M2 is a top-down conditioned Monte Carlo procedure, where households/dwellings are synthesized by Monte Carlo, families are conditionally synthesized on dwellings, and persons are conditionally synthesized on families. The results are evaluated on the person population only, to focus on the effects of the two stages of conditioning prior to generating the persons. The dwellings had ten attributes each, families had fifteen attributes (one shared with both dwellings and persons, four shared only with dwellings and two shared only with persons). The full set of input margins used are shown in Table 2. An overview of the M2 population synthesis procedure is shown in Figure 3. The numbered steps shown in the figure are (with compute times as indicated):

- 1. a. Fit households/dwellings using PUMS and Summary Tables with the multizone IPF procedure (30.4 minutes).
 - b. Fit persons using PUMS and Summary Tables (58.9 minutes).
- 2. Fit families using PUMS and Summary Tables; also fit to distributions of attributes shared with households/dwellings and persons (10.3 minutes).
- 3. Use Monte Carlo to synthesize a list of households/dwellings (0.9 minutes).
- 4. For each household/dwelling with one or more families, synthesize family/families conditioned on household/dwelling characteristics (3.6 minutes).
- 5. a. For each family, synthesize persons conditioned on family characteristics (10.9 minutes).
 - b. For each household/dwelling, synthesize non-family persons conditioned on household/dwelling characteristics (3.2 minutes).



Fig. 3 Overview of synthesis procedure. Numbers show the order of steps in the process. On the left, PUMS and Summary Table data are combined using a fitting procedure (Beckman et al.'s multizone IPF). On the right, Monte Carlo is used to synthesize a list of individual agents from the fitted tables, with conditioning included for families and persons.

As expected, the goodness-of-fit deteriorates after applying Monte Carlo, and deteriorates further using the conditional procedure. The deterioration from M0 to M1 is somewhat larger than the deterioration from M1 to M2. In essence, this shows that the conditional synthesis procedure employed here does not have a major impact on the goodness-of-fit. Even after two stages of conditioning (from dwellings to families to persons), a reasonable goodness-of-fit is maintained.

6.3 Implementation

The IPF routines were implemented using special-purpose software on the R statistical computing platform (Ihaka and Gentleman 1996) with a few routines in C. The total compute time for experiment M2 was two hours and seven minutes, running on an older 1.5 GHz computer with 2 GB of memory.

The data used for the experiments was the 1986 census of the Toronto Census Metropolitan Area (CMA). The census summary tables provide information about individual attributes in 731 census tracts (CTs) within the CMA, most of which are shown in Table 2. The associated PUMS datasets correspond to the entire CMA, and consist of:

- a 1% sample of 1120000 households and dwellings, with 10 of the available attributes used for each agent;
- a 1% sample of 906 385 families, with 15 attributes each;

The final synthesized population sizes are 100% of the populations above.

7 Conclusion

Two additions to the existing procedure for population synthesis have been proposed in this paper. The sparse storage technique yields clear advantages in memory usage for large numbers of attributes, while retaining all of the theoretical advantages of an IPF-based procedure. The conditional Monte Carlo synthesis procedure allows a simultaneous fit to household, family and person level data and permits a valid synthesis of relationships between agents for non-U.S. census data. The evaluation demonstrates that this conditional procedure has only a minor impact on goodness-of-fit relative to the conventional Monte Carlo approach.

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