Categorical Sequence Analysis with Optimal Matching: An Application with Data

from the 'Women 40+ Healthy Aging Study'

A Thesis

Presented to

The Division of Faculty of Science

University of Bern

In Partial Fulfillment

of the Requirements for the Degree

Master of Science in Statistics and Data Science

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June 2023

Approved for the Division
(Institute of Mathematical Statistics and Actuarial Science)

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Acknowledgements

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Abstract

In this work, we describe and use optimal matching (OM) — a method widely used in sociological studies — to obtain pairwise distances between categorical sequences that represent the relationship and family history of a group of women over 40 years old. We then use the distances to obtain clusters and predict five personality traits with k-nearest neighbors (k-NN) and compare the performance of different approaches using the mean squared error (MSE) of the prediction. The different approaches or scenarios are given by the calculation of the cost matrix, normalization and handling of missing values in the sequences. Our aim is to explore the effects that the variations considered in the scenarios have on an unsupervised and supervised distance-based method.

Dedication

A la memoria de mi Lunita.

Introduction

In order to extract useful information from a dataset of categorical sequences, we can obtain pair-wise distances between the data points and use a distance-based method which is particularly useful when dealing with complex data types. Depending on the objective of the researcher and the availability of other observed variables, we can apply an unsupervised or supervised learning technique. For example, we can obtain groups of similar sequences, identify common trajectories or predict other variables of interst.

In computational linguistics, we encounter several methods to obtain these distances, for instance, there is a category of measures known as *edit distances* that are widely used for text prediction. To give some examples, the Hamming distance accounts for differences at each time point or we can define a dissimilarity based on the length of common subsequences or prefixes. One of the measures considered as an edit distance is the Levenshtein distance which finds the minimum number of steps required to arrive to one sequence taking the other as a starting point. The steps can be insertion, deletions or substitutions in the case of the Levenshtein distance, but other distances also consider the option of character swaps.

In bioinformatics, a generalization of the Levenshtein distance was proposed by Needleman & Wunsch (1970) to find similarities in the amino acid sequences of two proteins. The Needleman-Wunsch algorithm finds the best alignment of two sequences by maximizing the similarity between them with the possibility of different penalization values for substitutions. This algorithm was introduced and adapted to social sciences by Abbott & Forrest (1986), who denominated it optimal matching (OM). Since then, it has been extensively used to answer questions involving sociological processes that take values in a categorical set and occur along a specific period of time, mainly in the study of paths of family formation or professional careers (see Abbott & Tsay (2000)).

One of the most common analysis strategy of several studies employing OM is to identify groups of trajectories that exhibit similar patterns based on the dissimilarities among categorical sequences. This is achieved through the application of clustering

techniques to the distance matrix generated with help of the algorithm. However, a variety of unsupervised and supervised learning techniques can be applied to the distance matrix obtained via OM depending on the particular research question addressed.

Furthermore, we want to draw special attention to the fact that, there are a number of decisions involved in the application of OM, namely the method for calculation of the *cost matrix* and their associated parameters or the normalization used to transform the distances to account for differences in their lengths. Moreover, we can interpret these decisions as hyperparameters that are subject to tunning.

In this work, we use a dataset that contains categorical sequences of the relationship and family formation history for a group of women. The time frame to be considered is from the age of 15 years to the current age at the time of data collection and the data was collected in the context of a larger research project denominated 'Women 40+ Healthy Aging Study'. The available data contains information about the civil status, relationship status, cohabitation status and maternity situation of the participants. In addition, the dataset encloses scores of personality traits that were obtained with a psychometric instrument.

Our aim it to explore the effect that changing the aforementioned hyperparameters has on the distance matrix obtained via OM. In the absence of a methodological framework to directly compare distance matrices, we consider the changes in the groups obtained via hierarchical clustering. On the other hand, we are interested in exploring the influence of the relationship and family history on the personality scores of the participants. For this purpose, we use a supervised learning technique and assess the quality of the prediction when the hyperparameters change.

One of he main tools to perform our investigation is the implementation of the OM algorithm in the `R` package `TraMineR` (Gabadinho, Ritschard, Müller, & Studer (2011)) as it provides several methods for data-based calculation of the cost matrix and functions to visualize categorical sequences.

The document is structured as follows: in Section 1 we give an account of the most commonly used edit distances, then we introduce the data we use in out application and explain the method chosen for prediction. In Section 2 we provide a detailed description of the optimal matching algorithm, including the methods considered to obtain the cost matrix and the normalization methods for the distance matrix. In Section 3, we provide more insight on the data and perform OM to obtain clusters of sequences and use visualizations to provide a description of the groups. In Section 4, we describe perform a first attempt at prediction of the personality scores based

on the data from the previous section and in Subsection 4.2, we show some of the additional scenarios considered, specifically those that produce the best predictions for each personality trait. Finally, we present some conclusions and recommendations for future work.

Section 1

Distance-based Methods for Categorical Sequences

Distance-based methods are a class of statistical techniques based on the use of distance, similarity or dissimilarity measure between data points instead of using the raw variables. The main idea behind these methods is to obtain a distance or dissimilarity matrix in order to apply an unsupervised or supervised learning method such as clustering in different variations, dimensionality reduction, multidimensional scaling or k-nearest neighbors (k-NN) when we are interested in using the data to predict other variable for which we have observed or labeled values.

Moreover, in case the available pair-wise distances are Euclidean, we can obtain centered inner products and this allows us to have several other techniques at our disposition, such as k-means clustering, multinomial regression, principal component anlaysis (PCA) ,linear discriminant analysis and support vector machines (SVM), see Hastie, Tibshirani, & Friedman (2009).

Distance-based methods have the advantage of allowing applications with a variety of data types, in particular, categorical sequences, i.e. sequences that take values in a finite set of categories or states and are indexed by time.

1.1 Distance Measures for Categorical Sequences

Several ways to compute distances between categorical sequences have been proposed in the context of natural language processing and bioinformatics. Particularly, a class of measures, known as *edit distances*, provide a quantification of the dissimilarity of a pair of sequences by counting the minimum number of operations required to obtain a sequence from the other. For instance, Hamming (1950) proposed a distance

for sequences of the same length that counts the number of positions with different states. Levenshtein (1966) generalized the Hamming distance to sequences of different lengths by considering the minimum number of single character edits required, namely insertion, deletion and substitution. The Damerau-Levenshtein distance allows for an additional operation known as transposition or swaping of characters (Damerau (1964)). The Jaro-Winkler similarity measure counts the number of matches and transpositions but does not fulfill the triangle inequality (Winkler (1990)). Additionally, there are several algorithms to find the longest common subsequence from a pair of subsequences (see Bergroth, Hakonen, & Raita (2000)), this could be seen as a measure that allows for insertion and deletion but not substitution nor transposition.

Also, note that from fundamental statistical methods for categorical data, considering the distribution of the states in a sequence, for a pair of sequences, the euclidean or χ^2 distance can be obtained and used in this context.

1.2   Optimal Matching and Applications

One generalization of the Levenshtein distance that allows for different substitution penalties for every pair of states is the Needleman-Wunsh algorithm, developed by Needleman & Wunsch (1970) with the aim of comparing and finding similarities between biological sequences (for example, DNA or protein sequences). This algorithm is an application of dynamic programming, an iterative method that simplifies an optimization problem by breaking it into a recursion of smaller problems that are simpler to solve. By choosing the optimal operation at each step, it is guaranteed that the overall solution is optimal as well. An adaptation of this algorithm that works with dissimilarities instead of similarities is known as *optimal matching* (OM), introduced in social sciences by Abbott & Forrest (1986) and widely applied in sociology. OM has been employed in several studies tracking the professional development of specific groups of people, see Chan (1995), Biemann & Datta (2014) or Gubler, Biemann, Tschopp, & Grote (2015), and to analyze life course data, for example, Widmer & Ritschard (2009) or Bastin (2015).

Limitations of OM have been pointed out by some critics. A notable flaw raised by Wu (2000) lies in the definition of the cost matrix — a core hyperparameter of the method — and the strong assumption about its symmetry. Initially, the method considered substitution costs that were provided by an expert in the context. However, data-based aproaches for the calculation of the cost matrix have been proposed since then, see Studer & Ritschard (2016).

Once a distance matrix has been obtained via OM or any other technique that is applicable to categorical sequences, a distance-based method can be used depending on the specific interest of the research. Usually, clusters are obtained in order to identify common trajectories through visual inspection, Abbott (1983) highlighted the possibility to use the distance matrix for multidimensional scaling, Gabadinho & Ritschard (2013) proposed a way to identify typical patterns based on the coverage neighborhood of the sequences applied to childbirth histories, Massoni, Olteanu, & Rousset (2009) combined OM and self-organizing maps in the study of career path and employability. In addition, Studer, Ritschard, Gabadinho, & Müller (2011) propose a methodology to analyze how covariates can explain the discrepancy between sequences based on their dissimilarities and Han & Moen (1999) used the groups obtained via clustering analysis of career trajectories to predict the age of retirement. However, to our knowledge, there has been no attempt at directly using categorical sequences for the prediction of other variables.

In this work we are interested in studying the effect of different hyperparameters when using OM to obtain pairwise distances of a group of sequences and subsequently employ them in distance-based methods. Particularly, we consider the effects on both clustering (unsupervised learning) and variable prediction with k-NN (supervised learning). For this purpose we analyze a new real-world dataset that includes categorical sequences, auxiliary information and other variables of interest: data from the "Women 40+ Healthy Aging Study".

1.3 Women 40+ Healthy Aging Study

As part of the Women 40+ Healthy Aging Study, a large study that was conducted by the Department of Clinical Psychology and Psychotherapy of the University of Zurich, a psychometric instrument was developed in order to obtain information about the history of romantic relationships of women: the categorical sequence of interest.

The study was conducted between June 2017 and February 2018 with women between 40 and 75 years who (self-)reported good, very good or excellent health condition and the absence of acute or chronic somatic disease or mental disorder. The participants who reported psychotherapy or psychopharmacological treatment in the previous 6 months, as well as habitual drinkers, were excluded. Other exclusion criteria were pregnancy in the last 6 months, premature menopause, surgical menopause, intake of hormonal treatment (including contraceptives), shift-work and recent long-distance flight. The participants were recruited from the general population using online

advertisement and flyers.

The questionnaire asked the participants to provide information about relationship phases starting from the age of 15 years until the current age at the time of the data collection. The phases were defined by the start and end age and for each phase and information about civil status, relationship status, living situation, children and quality of the relationship was collected. Before including the data corresponding to their own history, the participants were prompted to answer some of the questions based on an example. Some of the participants were excluded when the example entries were not correctly filled. After data cleaning and revisions for consistency the total number of individuals considered in this work is 239.

Additionally, personality scores for the women included in the study are available. Personality refers to the enduring characteristics and behavior that comprise the unique adjustment to life of a person, including major traits, interests, drives, values, self-concept, abilities, and emotional patterns. These scores are obtained via psychometric instruments and evaluate the main personality traits:

- Agreeableness
- Conscientiousness
- Extraversion
- Neuroticism
- Openness

One of our goals is to obtain groups of similar sequences that allow us to recognize typical relationship trajectories or behaviours of women over 40 years old. For this purpose, we apply a hierarchical agglomerative clustering analysis using Ward's method to minimize the dispersion within the clusters (Murtagh & Legendre (2014)), using the method `"ward.D2"` of the `hclust` function in `R`.

On the other hand, we want to understand the influence of relationship history of women on the personality scores which is of special interest for experts in psychology as there is a suspected association between the ability to maintain romantic relationships or having children and the dominant personality traits. The distance-based method chosen for prediction is k-NN, as for implementation we use the function `k.nearest.neighbors` from the `R` package `FastKNN`.

1.4   k-Nearest Neighbors

Let us remember that given a training set $\mathcal{D} = (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ of n labeled data points, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathcal{Y}$, a finite set of class labels for classification or a continuous range of values for regression. k-NN provides a way to predict the label or value for a new, data point x_{n+1} (for which y_{n+1} is unknown) by finding the k training data points closest to x_{n+1} and taking a majority vote of their labels (for classification) or averaging the values of Y (for regression). That is, for a given distance function $d(\cdot, \cdot)$ we predict y_{n+1} as:

$$\hat{y}_{n+1} = \frac{1}{k} \sum_{j=1}^{k} y_{(j)} \tag{1.1}$$

where $j = (1), \ldots, (k)$ index the nearest k neighbors of x_{n+1}:

$$d(x_{(1)}, x_{n+1}) < \cdots < d(x_{(k)}, x_{n+1}) < d(x_{(k+1)}, x_{n+1}) < \cdots < d(x_{(n)}, x_{n+1}) \tag{1.2}$$

There are different choices for the distance function $d(\cdot, \cdot)$. For instance, the Euclidean or Mahalanobis distances are common choices. In the case, of categorical sequences, we apply the more general OM algorithm to obtain a disimiliraty matrix.

In what follows we describe the OM algorithm in detail, including hyperparameters: the cost matrix and normalization functions.

Section 2

Optimal Matching Algorithm

As mentioned above, optimal matching is a technique widely applied in social sciences for the comparison of categorical sequences. OM uses the Needleman-Wunsch algorithm to identify similarities between biological sequences that are usually represented as strings of characters.

The goal of OM is to find the best possible alignment between two sequences by considering the differences and equivalences between their elements and minimizing the total cost associated. The cost of changing between states of the sequences we are interested in aligning, can be defined in several ways including data-based methods or values supplied by experts in the particular field.

Consider a set of n categorical states $S = \{s_1, \ldots, s_n\}$, we define $X = (x_1, \ldots, x_t)$, a sequence of length $t < \infty$, where $x_i \in S$ for $i = 1, \ldots, t$. Further, let $\mathbf{S}$ be the set of all possible sequences with states belonging to S.

Now, let $X, Y \in \mathbf{S}$ be two sequences of size t_X and t_Y, respectively. In order to numerically assess the disimilarity between the sequences X and Y, we define an empty array F of size $(t_X + 1) \times (t_Y + 1)$. Algorithm 1 below shows the initialization and recursion to fill the array F.

The value d is the cost of inserting a gap in one of the sequences, also known as *indel* cost, and $K(y_{i-1}, x_{j-1})$ is the cost associated to change from the state y_{i-1} to x_{j-1}, which is defined in a matrix K of size $n \times n$, commonly known as the cost matrix.

Lines 1-7 of the OM algorithm correspond to initialization. Starting with a cost of 0 in $F(1, 1)$, the first row and column of F represent cumulative costs of successively adding gaps. The remaining lines of the algorithm correspond to the row-wise recursion to fill the array F according to the content of the sequences to be compared: at any

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Algorithm 1 Optimal matching.

1: $F(1,1) \leftarrow 0$
2: **for** $j \leftarrow 2, t_Y + 1$ **do**
3:    $F(1,j) \leftarrow F(1,j-1) + d$
4: **end for**
5: **for** $i \leftarrow 2, t_X + 1$ **do**
6:    $F(i,1) \leftarrow F(i-1,1) + d$
7: **end for**
8: **for** $i \leftarrow 2, t_X + 1$ **do**
9:    **for** $j \leftarrow 2, t_Y + 1$ **do**
10:       $F(i,j) \leftarrow \min\{F(i-1,j)+d, F(i,j-1)+d, F(i-1,j-1)+K(y_{i-1}, x_{j-1})\}$
11:    **end for**
12: **end for**

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step of the recursion, the algorithm is looking at a specific pair of indexes (location) and calculating if substitution or insertion/deletion is the cheapest operation. Successively adding the costs of the cheapest operations results in the overall optimal cost for aligning the sequences X and Y.

In fact, when F is completely filled, the value in the last cell, i.e. $F(t_X + 1, t_Y + 1)$ corresponds to the minimal cost of aligning the sequences X and Y. It is possible to recover the steps that conduced to this alignment with a traceback from the last cell. However, this is not necessary to obtain the dissimilarities matrix for a set of sequences.

2.1 Example

Suppose that S is the alphabet and let $X = \{S, E, N, D\}$ and $Y = \{A, N, D\}$ be two sequences in **S**.

Further, let $d = 2$ and let $K(i,j)$ be the cost associated to change from state s_i to state s_j, for $i, j \in S$. This cost is given by:

$$K(i,j) = \begin{cases} 0 & \text{if } i = j, \\ 3 & \text{otherwise} \end{cases}$$

The array F is initialized as follows:

		S	E	N	D
	0	2	4	6	8
A	2				

	S	E	N	D
N	4			
D	6			

Then, to fill the second row of F we proceed as follows:

$$F(2,2) = \min\{F(1,2) + d, F(2,1) + d, F(1,1) + k(y_1, x_1)\}$$
$$= \min\{2 + 2, 2 + 2, 0 + 3\} = 3$$
$$F(2,3) = \min\{F(1,3) + d, F(2,2) + d, F(1,2) + k(y_1, x_2)\}$$
$$= \min\{4 + 2, 3 + 2, 2 + 3\} = 5$$
$$F(2,4) = \min\{F(1,4) + d, F(2,3) + d, F(1,3) + k(y_1, x_3)\}$$
$$= \min\{6 + 2, 5 + 2, 4 + 3\} = 7$$
$$F(2,5) = \min\{F(1,5) + d, F(2,4) + d, F(1,4) + k(y_1, x_4)\}$$
$$= \min\{8 + 2, 7 + 2, 6 + 3\} = 9$$

What yields:

		S	E	N	D
	0	2	4	6	8
A	2	3	5	7	9
N	4				
D	6				

Finally, after completing the recursion for the remaining rows, we obtain the following F array:

		S	E	N	D
	0	2	4	6	8
A	2	3	5	7	9
N	4	5	6	5	7
D	6	7	8	7	5

In this simple example, we can easily obtain two optimal (equivalent) alignments without using the algorithm:

S E N D with

A – N D or

– A N D

In both cases we have two matches (cost 0), one mismatch (cost 3) and one gap (cost 2), giving a total cost 5 that is exactly what we obtained in the last cell of F.

The cost of inserting a gap (d) is also known as *indel* (insert or delete) cost. In this example we can observe that, in order to obtain sequence X from Y we have to **insert** a term (i.e. insert a gap and then change its value to a specific state). Equivalently, to obtain sequence Y starting from X we have to **delete** one term.

The R packages `TraMineR` (Gabadinho et al. (2011)) and `TraMineRextras` provide several functions to define, analyze and visualize sequential data. In particular, `TraMineR` implements the OM algorithm and offers several methods for computing the cost matrix K and the normalization of the dissimilarity matrix.

2.2 Methods for Calculation of the Cost Matrix

The cost matrix K is a symmetric matrix of size $n \times n$. The value in the i-th row and j-th column $K(s_i, s_j)$ indicates the cost of moving from state s_i in time $t > 0$ to state s_j in $t + 1$.

The following are the methods available in `TraMineR` to obtain the cost matrix.

2.2.1 Transition rates (`TRATE`):

The substitution cost between states s_i and s_j, $1 \leq i, j \leq n$ is based on the observed relative frequencies of the transitions between the states and is calculated as:

$$K(s_i, s_j) = c - P(s_i|s_j) - P(s_j|s_i), \tag{2.1}$$

where $P(s_i|s_j)$ is the estimated probability of transition from state s_j in time t to s_i in time $t + 1$ and c is a constant, set to a value such that $0 \leq K(s_i, s_j) \leq 2)$.

The implementation of this method uses a default value of $c = 2$ which results in substitution costs that are close to 2. Additionally, as pointed out by Studer & Ritschard (2016), the calculation of substitution costs can lead to violations of the triangle inequality, meaning that we obtain a dissimilarity instead of a distance measure.

2.2.2   Chi-squared distance (`FUTURE`):

The χ^2-distance is a weighted sum of the squared differences of distribution vector frequencies. The weight is given by the inverse of the proportion of the total time spent in the state, meaning that the differences on rare states have higher weights.

$$K(s_i, s_j) = d_{\chi^2}(\mathbf{P_i}, \mathbf{P_j}) \tag{2.2}$$

$$= \left[\sum_{l=1}^{n} \alpha_l^{-1} \left(P(s_l|s_i) - P(s_l|s_i) \right)^2 \right]^{1/2} \tag{2.3}$$

where $\mathbf{P}_. = (P(s_1|s_.), \ldots, P(s_n|s_.))'$, and $\alpha_l = \sum_{h=1}^{n} P(s_l|s_n)$ and $i \neq j$.

It has been shown via simulation, that this distance is particularly sensitive to the time spent in each state but not so much to the order of the states in a sequence (see Studer & Ritschard (2016)).

2.2.3   Relative frequencies (`INDELS` and `INDELSLOG`):

$$K(s_i, s_j) = d_i + d_j, \tag{2.4}$$

where the *indel* cost d_i depends on the state and takes values:

$$g_i = \frac{1}{f_i}, \qquad\qquad \text{for method 'INDEL',} \tag{2.5}$$

$$g_i = \log\left(\frac{2}{1 + f_i}\right), \qquad\qquad \text{for method 'INDELSLOG'} \tag{2.6}$$

and f_i is the relative frequency of the state s_i for $i = 1, \ldots, n$.

Remarks:

- For methods `TRATE` and `FUTURE`, the unique *indel* value is $d = max_{1 \leq i,j \leq n} K(i,j)/2$, so that the cost of any change of state is always lower or equal than deleting and inserting an element (or vice versa). The reason behind is that higher *indel* costs, compared to the substitution costs, produce dissimilarities that are greatly affected by time shifts.
- The Needleman-Wunsch algorithm with constant costs for mismatch is known as Levenshtein distance (Levenshtein (1966)), a string metric widely used in computer science.
- In general, the resulting measure of the algorithm is a dissimilarity. However, if the cost matrix fulfills the triangle inequality, we obtain a distance measure (see

Yujian & Bo (2007)).

2.3   Normalization Methods for Distances

By design, OM can deal with sequences of different lengths via insertions. However, in cases when the lengths of the sequences differ greatly, it can be useful to account for this differences with a normalization factor.

Given a set two sequences $X, Y \in \mathbf{S}$ of length t_X and t_Y, respectively. Let $d(X, Y)$ be the dissimilarity between the sequences X and Y, t_{max} the length of the longest sequence in $\mathbf{S}$ and d_{max} the maximum dissimilarity between any pair of sequences in $\mathbf{S}$.

`TraMineR` offers the following options to normalize the dissimilarities between sequences:

- `maxlength`:
$$\frac{d(X, Y)}{t_{max}}$$

- `gmean`:
$$1 - \frac{d_{max} - d(X, Y)}{\sqrt{t_X * t_Y}}$$

- `maxdist`:
$$\frac{d(X, Y)}{d_{max}}$$

2.4   Example

Let $S = \{A, B, D, E, N, R, S\}$ and consider the following sequences in $\mathbf{S}$:

- $\{S, E, N, D\}$
- $\{A, N, D\}$
- $\{B, R, A, N, D\}$
- $\{B, R, E, A, D\}$
- $\{E, N, D\}$
- $\{R, E, D\}$
- $\{S, A, N, D\}$
- $\{D, E, A, N\}$
- $\{A, B, E, S\}$
- $\{N, A, B, E\}$

Table 2.4 shows the transition frequencies or estimated transition probabilities for the observed sequences. For this example, we observe a great amount of cells with the value 0 as there was no observed transition between those states. Additionally, the diagonal was set to 0 as we assume there is no cost associated with a match between two sequences.

Table 2.4: Observed transition frequencies.

	[-> A]	[-> B]	[-> D]	[-> E]	[-> N]	[-> R]	[-> S]
[A ->]	0.0000	0.2857	0.1429	0.0000	0.5714	0.0	0.0000
[B ->]	0.0000	0.0000	0.0000	0.5000	0.0000	0.5	0.0000
[D ->]	0.0000	0.0000	0.0000	1.0000	0.0000	0.0	0.0000
[E ->]	0.3333	0.0000	0.1667	0.0000	0.3333	0.0	0.1667
[N ->]	0.1667	0.0000	0.8333	0.0000	0.0000	0.0	0.0000
[R ->]	0.3333	0.0000	0.0000	0.6667	0.0000	0.0	0.0000
[S ->]	0.5000	0.0000	0.0000	0.5000	0.0000	0.0	0.0000

Now, suppose we want to obtain the cost matrix with the method `TRATE` with $c = 2$. We would procceed as follows:

$$K(A, B) = c - P(A|B) - P(B|A)$$
$$= 2 - 0.2857 - 0 = 1.7143$$
$$K(A, N) = c - P(A|N) - P(N|A)$$
$$= 2 - 0.5714 - 0.1667 = 1.2619$$

Table 2.5 shows the full cost matrix obtained from transition probabilities, which is a symmetric matrix. As we can observe, the positions values displayed in $K[1, 2], K[1, 2], K[1, 5], K[5, 1]$ are the same as those obtained above.

Table 2.5: Cost matrix obtained from transition probabilities.

	A	B	D	E	N	R	S
A	0.0000	1.7143	1.8571	1.6667	1.2619	1.6667	1.5000
B	1.7143	0.0000	2.0000	1.5000	2.0000	1.5000	2.0000
D	1.8571	2.0000	0.0000	0.8333	1.1667	2.0000	2.0000
E	1.6667	1.5000	0.8333	0.0000	1.6667	1.3333	1.3333
N	1.2619	2.0000	1.1667	1.6667	0.0000	2.0000	2.0000
R	1.6667	1.5000	2.0000	1.3333	2.0000	0.0000	2.0000
S	1.5000	2.0000	2.0000	1.3333	2.0000	2.0000	0.0000

Let us remember that in `TraMineR` the constant is set to 2 by default. 2.6 shows

the cost matrix obtained when we set the constant to 1.2, a value just above the maximum sum between the observed frequencies between states.

Table 2.6: Cost matrix obtained from transition probabilities with $c = 1.2$.

	A	B	D	E	N	R	S
A	0.0000	0.9143	1.0571	0.8667	0.4619	0.8667	0.7000
B	0.9143	0.0000	1.2000	0.7000	1.2000	0.7000	1.2000
D	1.0571	1.2000	0.0000	0.0333	0.3667	1.2000	1.2000
E	0.8667	0.7000	0.0333	0.0000	0.8667	0.5333	0.5333
N	0.4619	1.2000	0.3667	0.8667	0.0000	1.2000	1.2000
R	0.8667	0.7000	1.2000	0.5333	1.2000	0.0000	1.2000
S	0.7000	1.2000	1.2000	0.5333	1.2000	1.2000	0.0000

In addition to changing the value of c, we can opt for none or one of the normalization methods mentioned in the previous subsectionin order to obtain the distance matrix. Table 2.7 shows some descriptive statistics of the obtained distances for different methods of normalization.

Table 2.7: Comparison of descriptive statistics of the distances for different approaches of the cost matrix.

Normalization	Min	Max	Mean	Median	Std. deviation
None	1.0000	5.8333	3.6418	3.8333	1.2714
None / c=1.2	0.6000	3.0333	1.8920	1.8667	0.6144
'gmean'	0.1340	0.7113	0.4611	0.4783	0.1559
'maxdist'	0.1429	0.7143	0.4663	0.4815	0.1535
'maxlength'	0.2500	1.3750	0.8502	0.8667	0.2956

Section 3

Application of OM with Data from the 40+ Healthy Aging Study

As mentioned in Section 1, the dataset of interest contains data about the romantic and family history of a group of women. In order to create a sequence for each participant we condense the information about civil status, relationship status, cohabitational status and the maternity, i.e. presence or absence of children. For this purpose, and with the help of an expert, we analized the frequencies of the observed states for each sequence and simplified them according to their relevance. For instance, instead of considering widowed and divorced as separate states of the civil status, we only consider married or single (not married). Similarly, for relationship status we consider the states open relationship and same-sex relationship simply as being in a relationship given their low frequency. On the other hand, we simplified the number of children to a dichotomous variable that indicates if the woman has children or not.

Finally, the the four sequences are combined and we obtain a single yearly sequence, where the following states are considered:

- 1 = Single + no children
- 2 = Single + children
- 3 = Changing relationships + no children
- 4 = Changing rel. + children
- 5 = Relationship + living apart + no children
- 6 = Relationship + living together + no children
- 7 = Relationship + living apart + children
- 8 = Relationship + living together + children
- 9 = Married + no children

- 10 = Married + children

Figure 3.1 shows the overall distribution of states at each time point. We can observe that between ages 30 to 55 most of the women reported to be married and most of them also had children during those years. We can also observe that there is less variability after 60 years due to several missing values from this age as a consequence of the difference in lengths of the sequences.
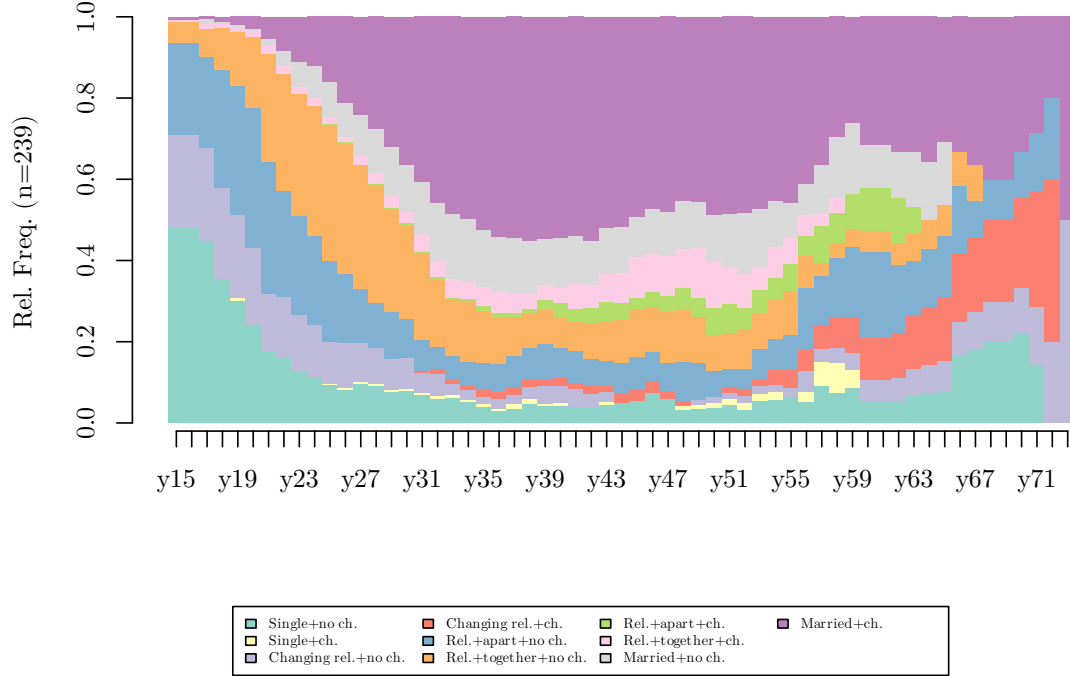

Figure 3.1: Cross-sectional distribution of relationship states.

Moreover, we want to explore potential relations between the personality and the categorical sequences. For instance, we subjectivelly define low or high levels of neuroticism as values on the lower or higher 20% of the distribution, respectively. Figure 3.2 shows that there is a higher variability in the observed states for women with high levels of neuroticism, while in the group of women with lower values of neuroticism, there is less variability of the observed states. This difference is particularly noticeable between the ages of 30 to 60 years.
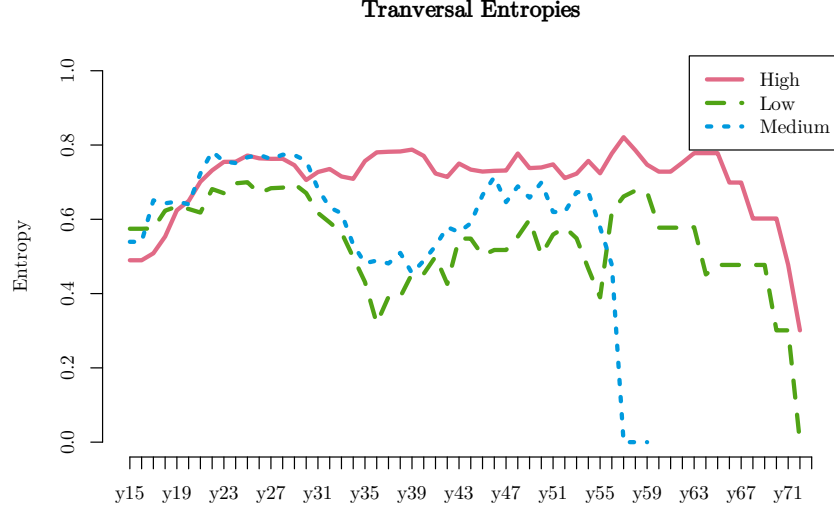
Figure 3.2: Transversal entropy for individuals with low or high levels of neuroticism.

3.1   Application of Optimal Matching

Using the `R` package `TraMineR` the cost matrix is calculated with transition rates between states. We consider a base setup with method `TRATE` for the calculation of the cost matrix and `maxlenght` normalization for the dissimilarities matrix, we name this the *base scenario*. The cost matrix obtained this way is shown in table 3.3.

Table 3.3: Cost matrix obtained from transition probabilities (method 'TRATE') of the relationship data of women over 40 years old.

State	1	2	3	4	5	6	7	8	9	10	NA
1	0.00	2.00	1.98	2.00	1.92	1.95	2.00	1.99	1.98	1.98	2
2	2.00	0.00	2.00	2.00	2.00	2.00	1.96	1.92	2.00	2.00	2
3	1.98	2.00	0.00	2.00	1.94	1.92	2.00	2.00	1.97	1.98	2
4	2.00	2.00	2.00	0.00	1.99	2.00	1.95	1.95	2.00	2.00	2
5	1.92	2.00	1.94	1.99	0.00	1.95	1.98	1.99	1.98	1.97	2
6	1.95	2.00	1.92	2.00	1.95	0.00	2.00	2.00	1.98	1.96	2
7	2.00	1.96	2.00	1.95	1.98	2.00	0.00	1.97	2.00	2.00	2
8	1.99	1.92	2.00	1.95	1.99	2.00	1.97	0.00	2.00	1.98	2
9	1.98	2.00	1.97	2.00	1.98	1.98	2.00	2.00	0.00	1.99	2
10	1.98	2.00	1.98	2.00	1.97	1.96	2.00	1.98	1.99	0.00	2
NA	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	0

As expected, the elements in the diagonal are equal to 0, meaning there is no cost associated to staying in the same state. By default, the constant c in 2.1 is set to 2. This, and the fact that the duration of the states is often longer than the time

unit (one year), makes that all of the values outside the diagonal are close to 2 and even equal in cases where no transition between the states were observed in the data (e.g. from single without children to single with children and vice versa). Finally, note that we consider missing value (`NA`) as a separate state and, by default, the cost of changing from or to a missing value is 2, which might be too high in cases where the individuals made a mistake in the beginning or end age of a phase leaving a gap in the sequence, or when the length of the sequences differ by a large number.

From this cost matrix it is possible to calculate pairwise dissimilarities between all the sequences using the optimal matching algorithm as described in the previous section. As stated before, a correction of the dissimilarities is done to account for the differences in length of the sequences, dividing the obtained dissimilarity by the length of the longest sequence.

Having obtained the dissimilarities matrix, we can derive the clusters with a hierarchical algorithm. Our aim is to explore the data and the differences captured by the dissimilarities matrix. In particular, we set the number of clusters to four, given that this is the maximum number of clusters that produces groups with meaningful differences in the distribution of states. Figure 3.4 shows the distribution of the states for each of the four identified clusters.
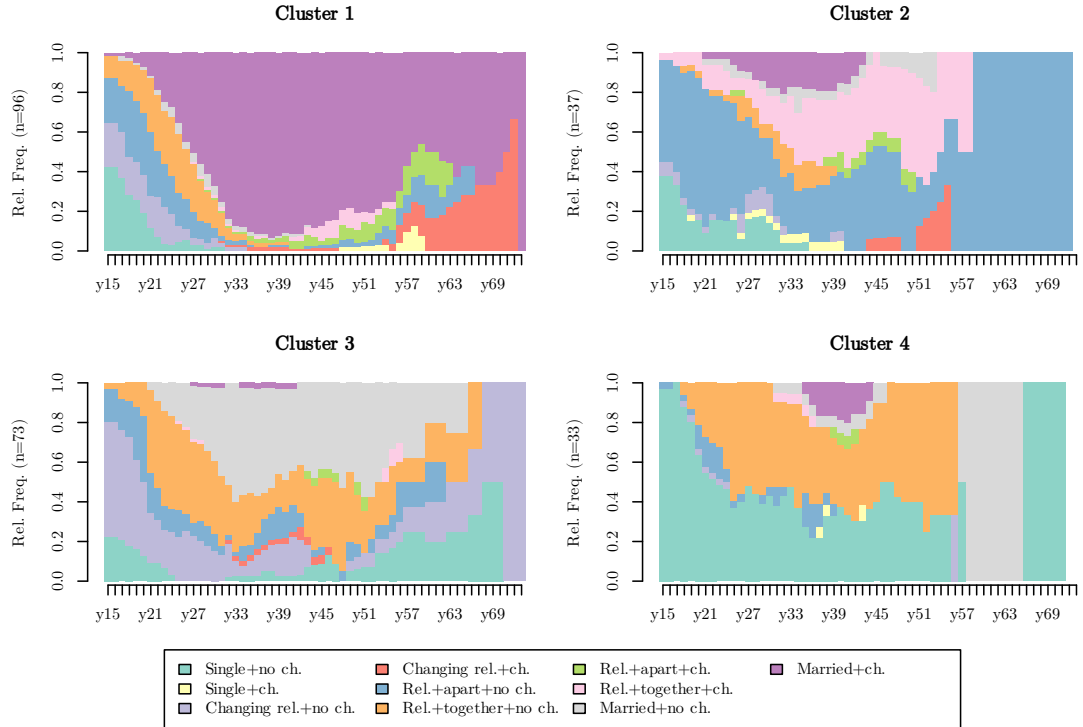

Figure 3.4: Cross-sectional distribution of relationship states by cluster for the base scenario.

In figure 3.5 we show the transverse entropy by cluster, i.e. the cross-sectional entropy of the states distributions is calculated at each time point as follows:

$$h(f_1, \ldots, f_n) = -\sum_{i=1}^{n} f_i \log(f_i), \qquad (3.1)$$

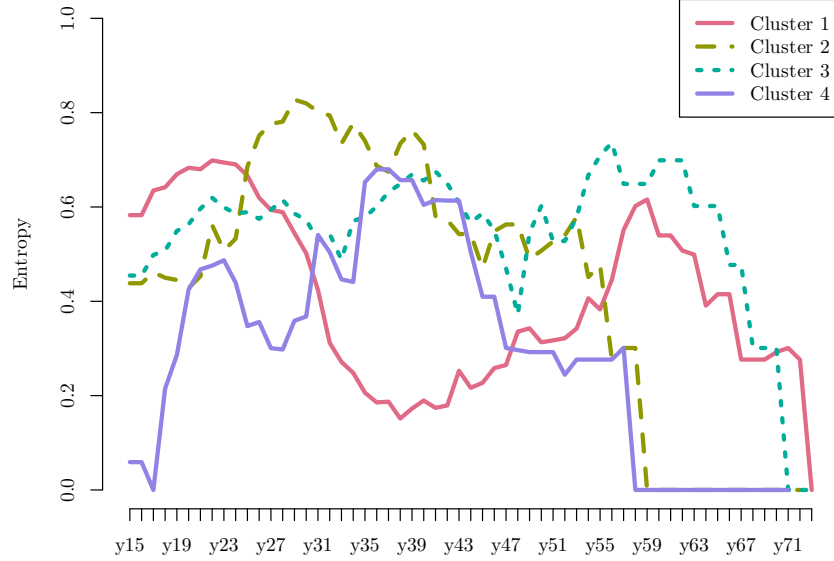where f_i is the relative frequency of state s_i.

Figure 3.5: Transversal entropy by cluster for the base scenario.

These visualizations allow us to identify common and contrasting features of the clusters that can be useful to describe them concisely. In table 3.6 we present a summary of the clusters with our descriptive interpretation of the clusters. It is important to remember that this descriptions are subjective and not exhaustive.

Table 3.6: Summary of the four clusters obtained in the base scenario.

Cluster	n	Share	Description
1	96	40.2%	Married young and had children.
2	37	15.5%	Often in relationships but not married.
3	73	30.5%	Older, mostly married or in long relationship without children.
4	33	13.8%	Younger, single or in a relationship without children.

On the other hand, in figure 3.4 we can also appreciate that the conformation of some clusters seems to be highly affected by the length of the sequence and it is reasonable to assume that the normalization method is not achieving the ideal result.

Now, we are interested in exploring how the relationships history of the women relate to personality traits. As a first exploratory step, figure 3.7 shows the distribution
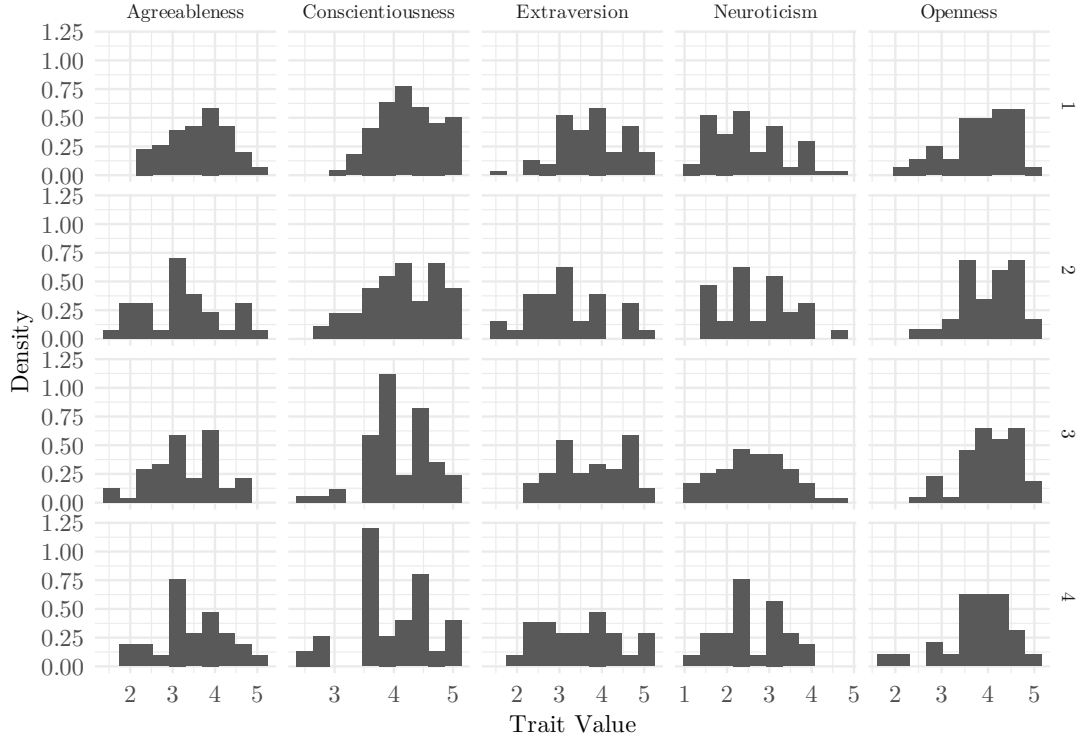
of the score for each trait by cluster.

Figure 3.7: Histogram of the five personality scores by cluster in the base scenario.

No difference is obvious at first glance. Also, the number of clusters and the fact that the personality scores are not continuous makes it difficult to identify differences. For that reason, we also explore with a lower number of clusters.

By setting the number of groups to only two, we obtain better defined clusters that are less affected by the length of the sequences as we can observe in the distribution plots of the sequences states (figure 3.8): the majority of women in cluster 1 have children, while we mostly find women without children in cluster 2.

In addition, the transversal entropy of the sequences for the two clusters is displayed in figure 3.9, where it is shown that the entropy decreases significantly around mid age for the cluster of women with children as compared to women without children, which means that the variability of the states for the first group is much lower as compared to the second group. This can be interpreted as a sign of stability in the relationship status for women during the time they have children at home.

On the other hand, Figure 3.10 shows the distribution of the sequences states at each time point when we calculate the cost matrix with method `TRATE` but change the value of the constant c to the maximum value of the sum of the transition
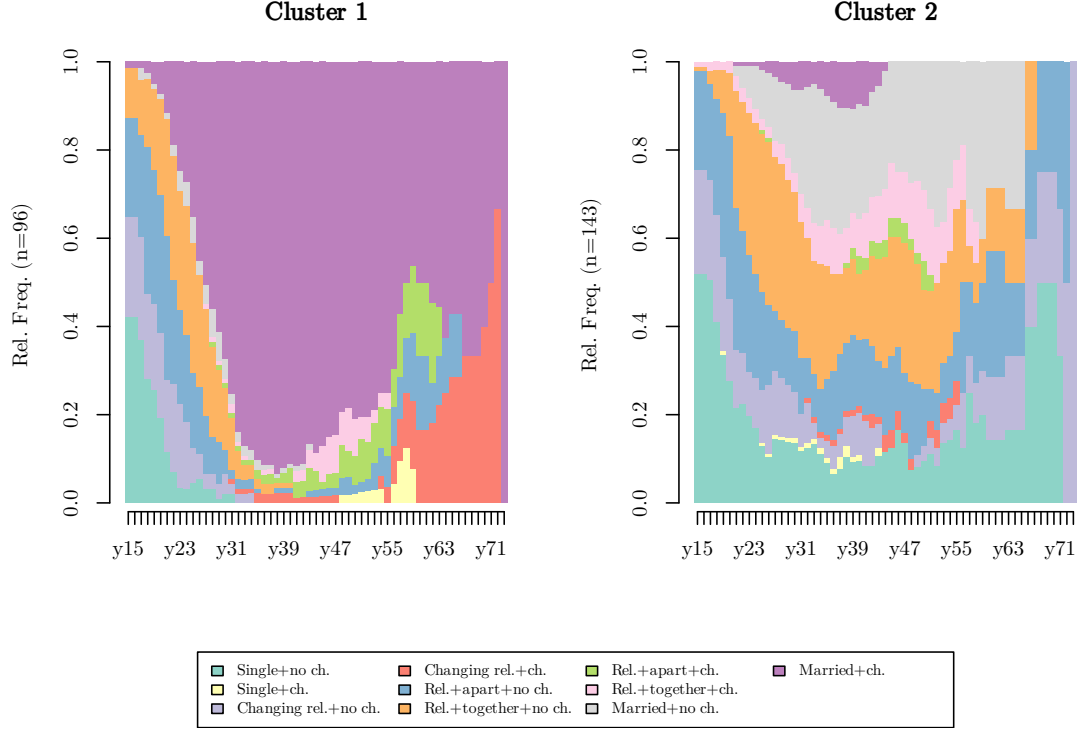
Figure 3.8: Cross-sectional distribution of states for two clusters in the base scenario.

frequencies between pairs of states. Also, Figure 3.11 shows the distribution of the sequences states at each time point when we calculate the cost matrix with method `FUTURE` and use the method `gmean` for the normalization of the distances between the categorical sequences. In both cases, by visual inspection, we obtain clusters that show cross-sectional distributions of the states that are very similar to the base scenario.

As mentioned before, we want to explore possible links between the information from the sequences and personality scores. For this reason, we display in Figure 3.12 the distribution of the personality traits for the two clusters. There seems to be differences in the distributions of some personality scores: the scores of agreeableness are concentrated in larger values for women with children; women without children have greater frequency in lower values of conscientiousness than women with children; and women with children exhibit lower scores of neuroticism.

Even though, the distribution of personality scores by cluster does not reveal significant differences, having a dissimilarity matrix provides a numerical expression of the categorical sequences that is useful for other purposes. In particular, in the next section, we explore the predictive capability of this dataset using a non-parametric prediction method.

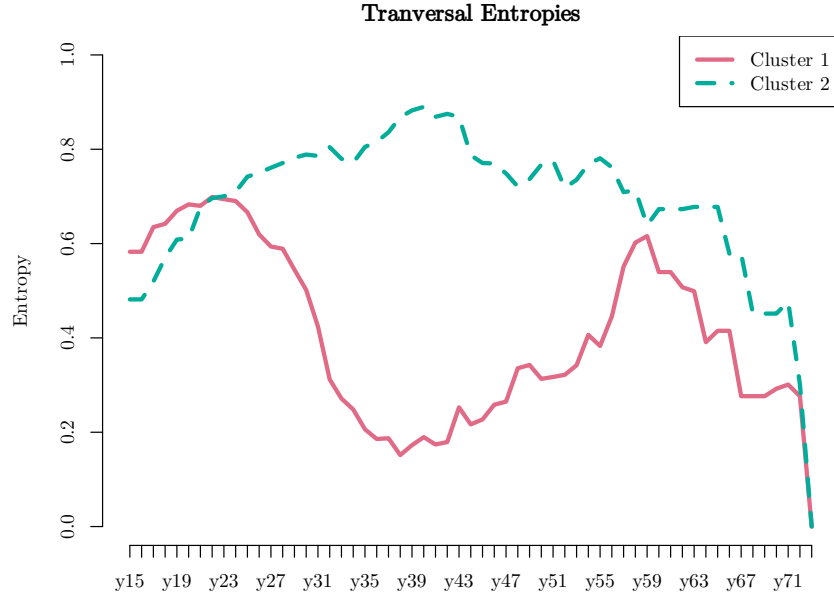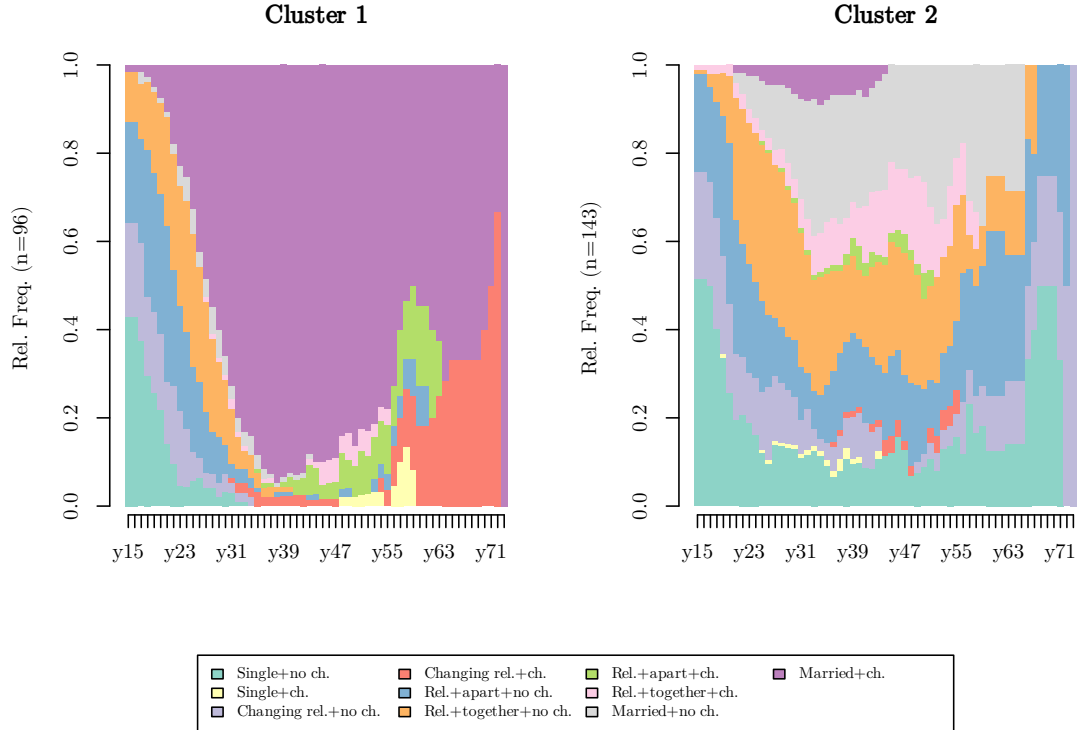Figure 3.9: Transversal entropy for two clusters in the base scenario.

Figure 3.10: Cross-sectional distribution of states for two clusters changing the value of c.
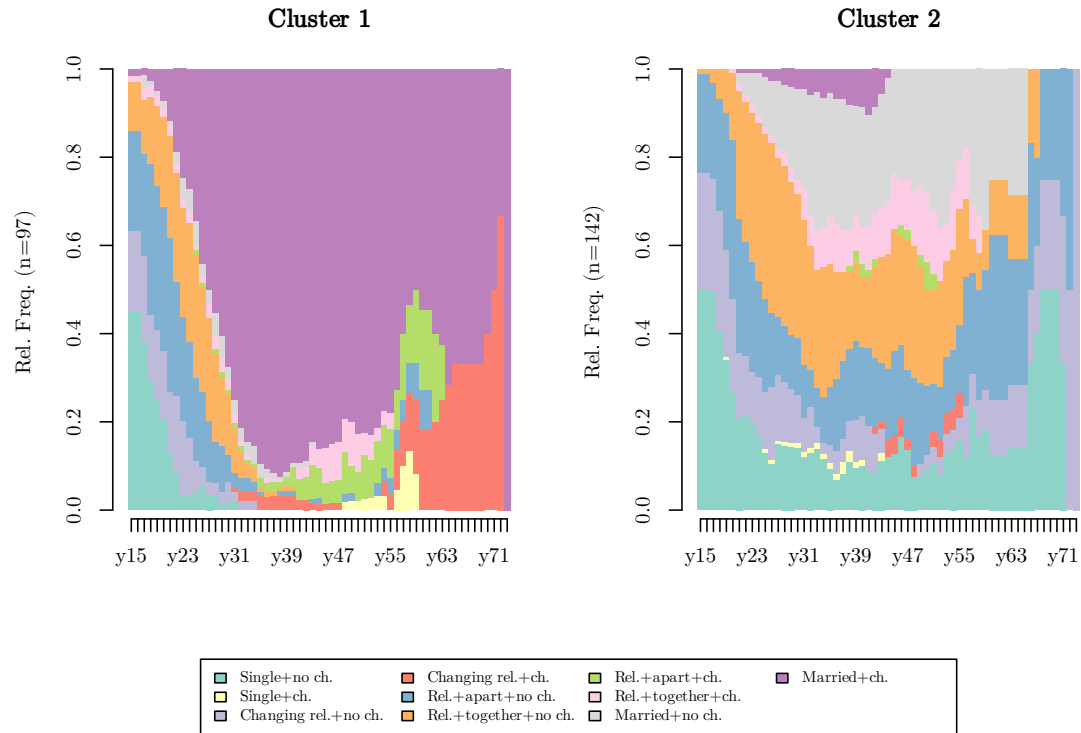
Figure 3.11: Cross-sectional distribution of states for two clusters with method 'FUTURE' forcost matrix calculation and method 'gmean' for distances normalization.
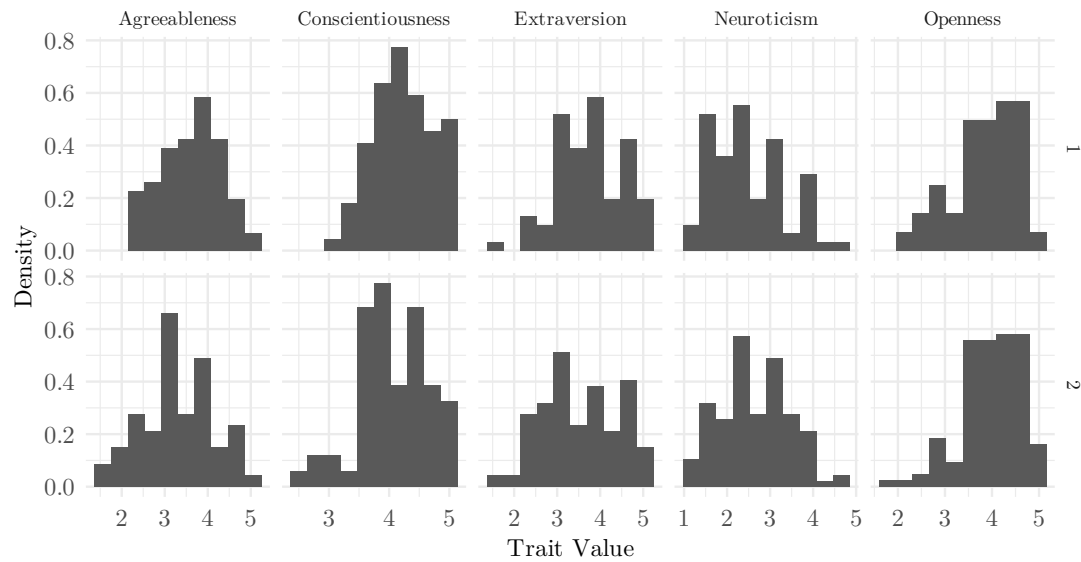

Figure 3.12: Histogram of the five personality scores for two clusters in the base scenario.

Section 4

Personality Scores Prediction with k-NN

Our interest in this section is to obtain predictions of the scores on the five personality traits using the information contained in the sequences of relationship and family history as a predictor. The reason behind this is the supposition that the type and duration of romantic relationships of a person and later on the maternity has an impact on their personality. For example, we hypothesize that parents may display more extraversion as they interact with other parents or single people can show more openness to new experiences.

As for the method to obtain the predictions we have opted for k-NN as it is easily implemented from a distance or dissimilarity matrix and does not make any assumption about the (conditional) distribution of the response variables. Note that in this setup, $d(\cdot, \cdot)$ is one of the multiple normalized dissimilarities $d(\cdot, \cdot) = d'(\cdot, \cdot | K)$ and it is dependent or parametrized by the cost matrix K.

Furthermore, k is also a hyperparameter that can be tuned to optimize the performance of the k-NN algorithm. A larger k reduces the effect of noise and outliers but can also lead to overfitting. A smaller k is more sensitive to noise and outliers but can capture better the local structure.

To compare the performance of different values of k and other hyperparameters, we use the mean squared error (MSE). For a testing set of m labeled data points, the MSE is given by:

$$\text{MSE} = \frac{1}{m} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 \tag{4.1}$$

where y_i is the observed value and $\hat{Y}_i$ is the predicted value via kNN.

4.1 Personality Scores Prediction in the Base Scenario

In this part of the analysis we only consider the individuals who have available personality scores, that results in a sample size of 200 individuals. Additionally, we randomly split the data into two subsets: train (70%) and test (30%) and we evaluate the MSE of the predictions for the individuals in the test set only using the data from the nearest neighbors available in the train set.

For each trait we predict the personality score values Y and compare them with the observed values using the MSE. Table 4.1 summarizes the results of the optimal prediction and Figure 4.2 shows the MSE for the different values of k, i.e. for $k = 1, \ldots, 80$. As a reference, a red line for every personality trait is added to indicate the MSE of the trivial prediction, i.e. the mean of all the sample points in the train set. Recall that we are using the cost matrix K shown in Table 3.3 and normalized dissimilarity defined by the `maxlength` method as described in Subsection 3.1.

Table 4.1: Summary of k-nn prediction of personality scores in the base scenario.

Trait	min(MSE)	k	Trivial MSE
Agreeableness	0.59	48	0.62
Conscientiousness	0.37	15	0.40
Extraversion	0.71	22	0.76
Neuroticism	0.64	7	0.71
Openness	0.54	12	0.54

Overall, it seems that using the sequential data for prediction results in little improvement compared to the trivial prediction. For neuroticism, the MSE decreases rapidly, reaching the lowest value at $k = NA$ and then increases again.

Furthermore, for conscientiousness and openness, the MSE does not seem to increase again as k increases, which is expected when using kNN, due to overfitting. Moreover, for openness, the prediction with kNN is always worse than the trivial prediction. For conscientiousness, the MSE takes a minimum value for $k = 15$ and after $k = 30$ the MSE curve stays flat.

For agreeableness, the MSE increases again after the optimal k. However, note that this minimum is not considerably lower than the trivial prediction. Similarly, for extraversion, the MSE takes a minimum value with $k = 22$, but is not a significant improvement compared to the trivial prediction.
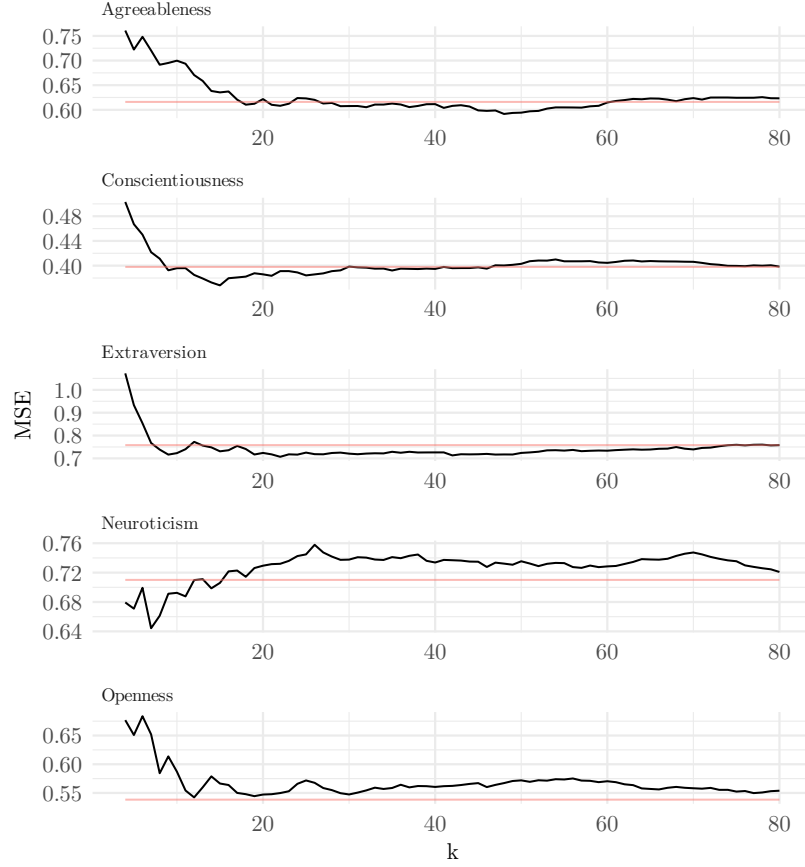
Figure 4.2: Prediction MSE by personality trait in the base scenario with trivial prediction reference (red line).

Given that the performance of the predictions is just slightly better than average in most cases, we contemplate other scenarios with different variations of the hyperparameters considered in this section, namely the cost matrix and choice of normalized dissimilarity.

4.2 Additional Scenarios Considered for Prediction

In order to assess the imparc of the hyperparameters and find better predictions for the personality scores, we considered different configurations for obtaining the cost and dissimilarity matrices. For instance:

- Take the constant c in 2.1 as $2 * max_{1 \leq i,j \leq n} P(i,j)$ so that $0 \leq K(s_i, s_j) \leq 2 * max_{1 \leq i,j \leq n} P(i,j) \leq 2$.

- Consider the methods `FUTURE`, `INDELS` and `INDELSLOG` for the calculation of the cost matrix.

- Try `gmean` and `maxdist` as the normalization factor for the distance matrix.

- Consider several values from 0 to 2 for the transition from/to missing value, given that this has a significant effect when comparing sequences with large differences in length. Also, we can appreciate this effect in the conformation of the clusters (see Figure 3.4).

- Given that the previous consideration resulted in better prediction performance, and with the aim of obtaining more homogeneous sequences in length, we limit the start and end age of the sequences.

Table 4.3 shows the configuration of some of the scenarios considered for prediction.

Table 4.3: Summary of additional scenarios considered for obtaining dissimilarity matrix.

	Cost matrix	Normalization	Transition constant	NA cost	Min age	Max age
1	TRATE	maxlength	NULL	NULL	NULL	NULL
2	TRATE	maxlength	0.08021433	NULL	NULL	NULL
3	TRATE	gmean	0.08021433	NULL	NULL	NULL
4	FUTURE	maxlength	NULL	NULL	NULL	NULL
5	INDELS	maxlength	NULL	NULL	NULL	NULL
6	INDELSLOG	maxlength	NULL	NULL	NULL	NULL
7	FUTURE	gmean	NULL	NULL	NULL	NULL
8	FUTURE	maxdist	NULL	NULL	NULL	NULL
9	FUTURE	gmean	NULL	1	NULL	NULL
10	FUTURE	gmean	NULL	NULL	20	55
11	FUTURE	gmean	NULL	NULL	20	40
12	FUTURE	gmean	NULL	1	20	55
13	FUTURE	gmean	NULL	0.5	20	55

With the purpose of comparing the predictions obtained with the different scenarios, we calculate the relative improvement (p) compared to the trivial prediction for each value of k and each scenario.

$$p = (1 - (MSE_k/MSE_{trivial})) * 100 \tag{4.2}$$

Figure 4.4 shows the best relative improvement achieved for each personality trait and under all the scenarios in 4.3 and the corresponding value of k at which the best performance was obtained.

We can observe high variability in the prediction improvement when the scenario changes, which shows a high dependency of the predictions and hence of the distances
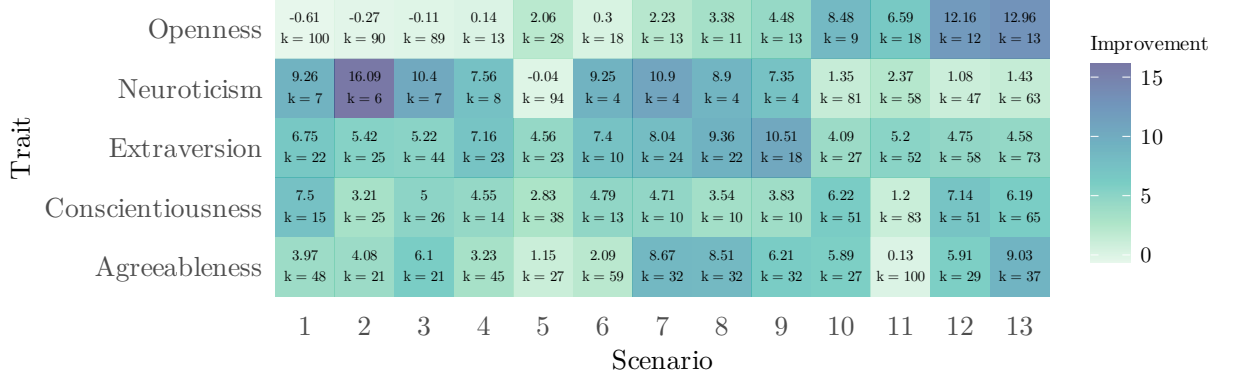
Figure 4.4: Improvement of MSE in the prediction of personality scores relative to the trivial prediction and respective value of k for each scenario.

on the hyperparameters. Although there is not a single scenario that produces the best prediction improvement for every trait, the method `FUTURE` seems to produce better results for all of the traits except neuroticism. On the other hand, method `INDELS` consistently yields poor quality predictions.

Figure 4.5 shows the MSE for neuroticism in scenario 2 in which the cost matrix is calculated with transition rates, the normalization method for the distances is `maxlength` and the constant c was modified. Also, we observe that for this particular trait, the configurations that aim to reduce the effects of missing values produce low improvements in prediction.
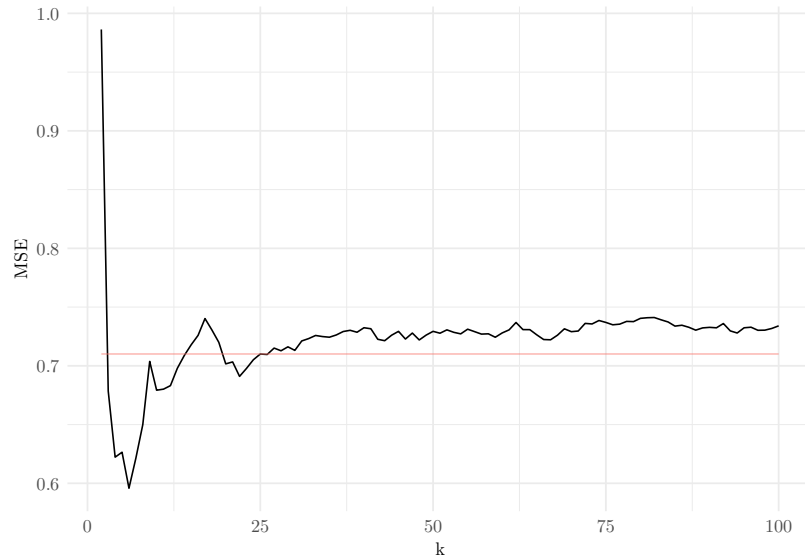

Figure 4.5: MSE of neuroticism prediction with trivial prediction MSE as reference (red line) in scenario 2.

We can observe that the best prediction is achieved at $k = 6$. However, the MSE at this point is much lower than the rest of the curve. It might be the case that this is a random occurrence. However, in 4.4 we observe the minimum MSE is found with a similar number of neighbors for other scenarios, for instance, in scenario 3 (see Figure 4.6).
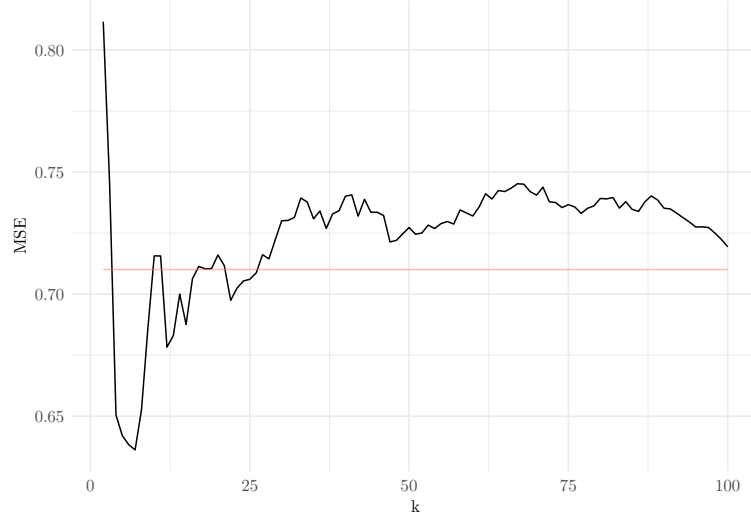

Figure 4.6: MSE of neuroticism prediction with trivial prediction MSE as reference (red line) in scenario 3.

For openness, the best predictions are obtained with scenarios 12 and 13. In both scenarios the cost matrix is calculated with χ^2 distance of the states frequencies (method FUTURE), normalization with the method gmean and the sequences are restricted between 20 and 55 years of age. This scenarios differ in the cost assigned to changes involving missing values. Hence, we might infer that the prediction of openness is highly affected by the way missing values are handled. Figure 4.7 shows the MSE for openness in scenario 13.

In the case of openness, we observe that the curve is lower around the values near to where the minimum is obtained at $k = 13$ and it increases to values where the performance is worst than the trivial prediction from $k > 25$.

The scenario that produces the best prediction for extraversion is number 9 and, similarly to neuroticism, is not favoured by configurations that aim to reduce the effects of missing values. In Figure 4.8, the MSE for scenario 9 is shown. This scenario was obtained with method FUTURE and a missing value transition cost of 1 for obtaining the cost matrix, and the distances were normalized with method gmean.

For extraversion, the minimum MSE is obtained when $k = 18$ which is a high number of neighbors compared to the two previous traits. As expected, the MSE
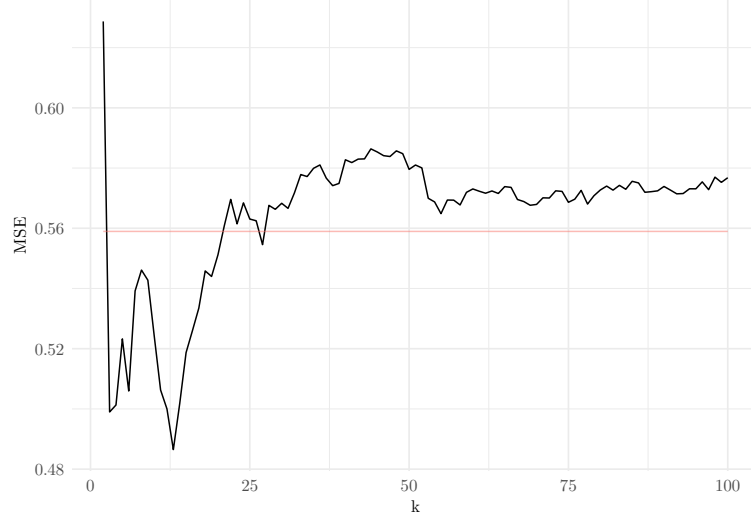
Figure 4.7: MSE of openness prediction with trivial prediction MSE as reference (red line) in scenario 13.

decreases until this value and then starts to increase again, a sign of overfitting for bigger values of k.

For conscientiousness none of the predictions achieved a relative improvement of at least 10%. Furthermore, the best prediction is obtained for $k = 15$ in the base scenario. Scenario 12 produces a similar result in terms of improvement, but with $k = 51$ which is an undesirable high number of neighbors for prediction with kNN. Figure 4.9 shows in detail the MSE for conscientiousness in the base scenario.

Likewise, for agreeableness, all of the scenarios showed improvements relative to the trivial prediction that are below 10% and the minimum MSE in every case is obtained for rather large values of k. This could be an indication of poor predictive power of the relationships history of women for this particular trait. However, as expected for this prediction technique, we observe in Figure 4.10 that the MSE is large and even greater than the MSE of the trivial prediction for values of k below 25 and after achieving the minimum it starts increasing again.

Finally, we perform clustering again with the distance matrix obtained in Scenario 13. Table 4.11 shows the cost matrix for this setup of parameters.

We can appreciate that in this case the range of the values of the cost matrix (excluding the diagonal elements and the missing value cost) is larger than those observe in 3.3. Figure 4.12 shows the distribution of states by cluster for this scenario.

Even tough the cost matrix presented large variations compared to the base scenario and the predictions improved, we obtain clusters that exhibit similar main
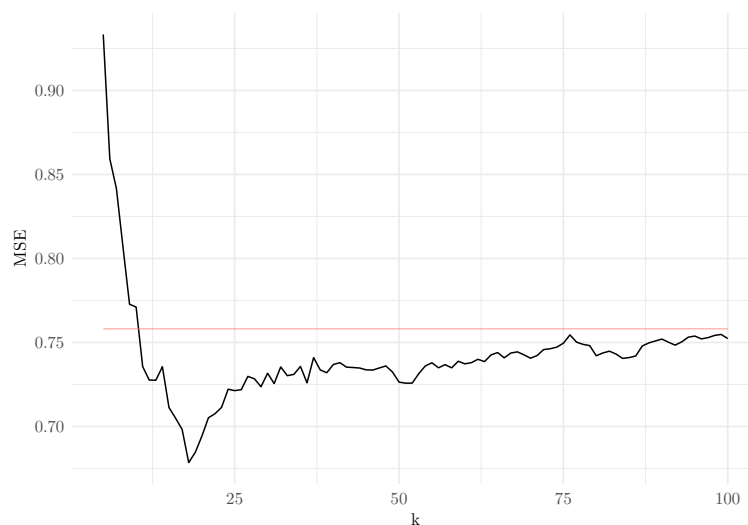
Figure 4.8: MSE of extraversion prediction with trivial prediction MSE as reference (red line) in scenario 9.

characteristics: In cluster 1, we find women with different relationship situations but without children. Similarly, in cluster 2 we find women with different relationship trajectories, but mostly married, that eventually had children. The clusters seem to be better defined in this case but that can be also due to the age restriction imposed, which implies that some sequences without enough data in the specified age range were excluded.

Figure 4.9: MSE of conscientiousness prediction with trivial prediction MSE as reference (red line) in scenario 2.

Figure 4.10: MSE of agreeableness prediction with trivial prediction MSE as reference (red line) in scenario 13.

Table 4.11: Cost matrix for scenario 13: sequences restricted to ages from 20 to 55, cost from/to missing value of 0.5, method for calculation of cost matrix 'FUTURE' and dissimilarity normalization 'gmean'.

| State	1	2	3	4	5	6	7	8	9	10	NA
1	0.00	1.31	1.24	1.28	1.18	1.18	1.25	1.26	1.28	1.25	0.5
2	1.31	0.00	1.30	1.33	1.28	1.28	1.27	1.32	1.34	1.33	0.5
3	1.24	1.30	0.00	1.27	1.17	1.14	1.24	1.26	1.26	1.23	0.5
4	1.28	1.33	1.27	0.00	1.25	1.24	1.22	1.24	1.31	1.29	0.5
5	1.18	1.28	1.17	1.25	0.00	1.15	1.20	1.24	1.24	1.22	0.5
6	1.18	1.28	1.14	1.24	1.15	0.00	1.21	1.23	1.23	1.20	0.5
7	1.25	1.27	1.24	1.22	1.20	1.21	0.00	1.24	1.28	1.26	0.5
8	1.26	1.32	1.26	1.24	1.24	1.23	1.24	0.00	1.31	1.28	0.5
9	1.28	1.34	1.26	1.31	1.24	1.23	1.28	1.31	0.00	1.30	0.5
10	1.25	1.33	1.23	1.29	1.22	1.20	1.26	1.28	1.30	0.00	0.5
NA	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.0
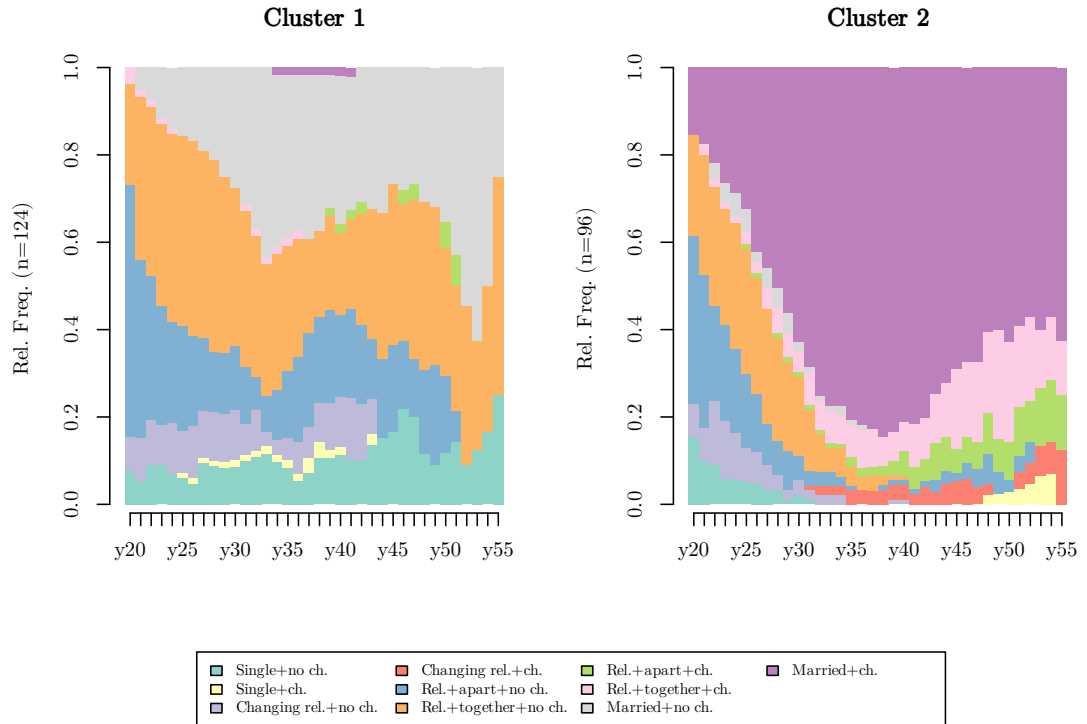
Figure 4.12: Cross-sectional distribution of states for two clusters in Scenario 13.

Conclusion

The use of optimal matching to calculate distances for categorical sequences in the context of social studies has been extensively documented. Many of these applications use the distance matrix obtained via OM as an input for an unsupervised learning technique, such as clustering or multidimensional scaling. Furthermore, this exercise implies a number of considerations in the calculation of the cost matrix and normalization of the distances. We consider these decisions and the ones concerning the handling of missing values as hyperparameters that are subject to tuning.

With a dataset of categorical sequences that contain information about the relationship and family history of a group of women we performed OM and obtained clusters that allow us to identify the most usual trajectories.dditionally, we explored the potential to use the resulting distance matrix for the prediction of personality traits scores with k-NN; note that we are adding another hyperparameter to our analysis, namely k. We decided to use MSE to evaluate the performance of the predictions under different scenarios, i.e. combinations of hyperparameters.

Based on the analysis of MSE obtained in different scenarios, we have determined that there is not a single specific combination of cost matrix generation method, normalization method, and treatment of missing values that consistently yields the best prediction for personality scores. However, when it comes to most personality traits, it is preferable to use the cost matrix calculated with the χ^2-distance of the states frequencies.

We also noted that the difference in sequence lengths affected the performance of the prediction as this produced a large amount of missing values, showing the limitation of any normalization method used.

Furthermore, we also observed that in the two scenarios that we considered for clustering, the resulting states distributions when dividing the individuals into two clusters, show that the main differentiating factor between them is the presence or absence of children (see Figure 3.8 and Figure 4.12).

It is worth noting that critics of this technique have pointed out that the results

heavily rely on how the cost matrix is defined and we have confirmed this with the results of the prediction performance. However, when it comes to unsupervised learning, the results seem to be more robust, except for methods `INDELS` and `INDELSLOG` that produced unidentifiable clusters.

As for future work, we consider that it would be convenient to consider another method for obtaining the cost matrix. For instance, in the specific context of the relationship history, it makes sense to consider an asymmetrical cost matrix as it is likely that the change from one state to another is more frequent that the converse. We also recommend a cross-validation approach for a more robust comparison of the scenarios. Additionally, it would be ideal to count with an objective measure for the comparison of the clusters obtained and consider other techniques for unsupervised learning. Finally, if it can be shown that the distances obtained are Euclidean, we could use other methods that yield better predictions.

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