# Fast algorithms to generate individualized designs for the mixed logit choice model

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Submission for track:
D: Activity and Transport Demand Analysis
D4: Data collection methods

# 1 Introduction

Efficient design of discrete choice experiments is essential to obtain precise estimates for the coefficients in the choice models. We assume that the choice behavior can be represented by the mixed (or random coefficients) logit choice model. As parameters are estimated at the individual level, the mixed logit choice model mirrors real choice behavior better.

As the generation of an aggregate efficient design for the mixed logit choice is computationally cumbersome (cfr Bliemer and Rose, 2010), Yu et al. (2011) introduced individualized Bayesian $\mathcal{D}$-efficient designs to elicit choice data for the mixed logit choice model. Individualized choice designs are sequentially generated for each person separately by summarizing the answers to previous choice sets as prior information to efficiently select the next best set. They are shown to yield more efficient estimates for the mixed logit choice model than an aggregate design optimized for a simpler model (Danthurebandara et al., 2011; Yu et al., 2011).

Despite the increasing computational capacity of modern computers, the generation of the next $D$-efficient choice set still takes seconds for small settings. This paper presents new design criteria that have been used in optimal test design to construct individually adapted choice designs for the mixed logit choice model and compares them with the $\mathcal{D}$-efficiency criterion that has often been used is this context.

Recently, three novel selection rules, based on Kullback-Leibler information, have been introduced in the test design literature. For individualized test design, the new criteria have been shown to be very useful. In this paper we apply the Kullback-Leibler criteria to design individualized choice experiments. Their implementation in a discrete choice setting is shown to be efficient and very fast.

# 2 Methodology

## 2.1 The mixed logit choice model

In a discrete choice experiment respondents must choose their preferred travel option in a series of choice sets contrasting multiple alternatives. The mixed logit choice model probability that a person $n$ chooses alternative $k$ in choice set $s$ (with $K$ alternatives) equals

$$p_{ksn}(\boldsymbol{\beta}_n) = \frac{e^{\mathbf{x}'_{ksn}\boldsymbol{\beta}_n}}{\sum_{i=1}^{K} e^{\mathbf{x}'_{isn}\boldsymbol{\beta}_n}}, \tag{1}$$

with $\mathbf{x}_{ksn}$ and $\boldsymbol{\beta}_n$ both $p$-dimensional vectors representing respectively the attribute levels of the $k$th alternative and individual $n$'s coefficients.

Conditional on $\boldsymbol{\beta}_n$ and given the choice design $\mathbf{X}_n^S$ with $S$ choice sets and corresponding choices $\mathbf{y}_n^S$, the likelihood of the model for respondent $n$ is thus given by

$$L(\boldsymbol{\beta}_n|\mathbf{y}_n^S, \mathbf{X}_n^S) = \prod_{s=1}^{S}\prod_{k=1}^{K}[p_{ksn}(\boldsymbol{\beta}_n)]^{y_{ksn}}, \tag{2}$$

with $\mathbf{X}_n^S = (\mathbf{x}'_{11n}, ..., \mathbf{x}'_{K1n}, ..., \mathbf{x}'_{KSn})'$ the design matrix stacking the attribute levels of all profiles in the choice experiment and vector $\mathbf{y}_n^S$ comprising the elements $y_{ksn}$ which are 1 if person $n$ chooses alternative $k$ in choice set $s$ and zero otherwise.

To model the aggregate choice behavior in the population the mixed logit choice model assumes a heterogeneity distribution, in most cases a multivariate normal distribution, over the individual-specific coefficients:

$$\boldsymbol{\beta}_n \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}). \tag{3}$$

The unconditional likelihood for respondent $n$ then equals

$$L(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathbf{y}_n^S, \mathbf{X}_n^S) = \int L(\boldsymbol{\beta}_n|\mathbf{y}_n^S, \mathbf{X}_n^S)\ \phi(\boldsymbol{\beta}_n|\boldsymbol{\mu}, \boldsymbol{\Sigma})\ d\boldsymbol{\beta}_n, \tag{4}$$

with $\phi$ the normal density.

## 2.2 Efficient individualized design for the mixed logit choice model

Here we discuss the algorithms to construct individualized choice designs for the mixed logit choice model based on either $\mathcal{D}$-efficiency or Kullback-Leibler information.

### 2.2.1 Minimum posterior weighted $\mathcal{D}$-error: a Fisher information design criterion

$\mathcal{D}$-efficient designs minimize the generalized variance of the parameter estimates (Atkinson et al., 2007). Assuming Bayesian estimation, the logarithm of the posterior will be used here instead of the logarithm of the likelihood yielding a Bayesian Fisher information matrix (BFIM). Given a design $\mathbf{X}_n^S$ for respondent $n$ and assuming a multivariate normal prior with covariance matrix $\boldsymbol{\Sigma}_0$, the Bayesian Fisher information matrix becomes

$$\mathbf{I}_{BFIM}(\boldsymbol{\beta}_n, \mathbf{X}_n^S) \;\; = \;\; \sum_{s=1}^{S}\mathbf{X}'_{sn}(\mathbf{P}_{sn} - \mathbf{p}_{sn}\mathbf{p}'_{sn})\mathbf{X}_{sn} + \boldsymbol{\Sigma}_0^{-1}, \tag{5}$$

with $\mathbf{X}_{sn}$ the design matrix of choice set $s$, $\mathbf{P}_{sn} = \mathrm{diag}(p_{1sn}, ..., p_{Ksn})$ and $\mathbf{p}_{sn} = (p_{1sn}, ..., p_{Ksn})'$.

Instead of maximizing the determinant of this information matrix, we minimize the inverse, denoted as the $\mathcal{D}$-error and proportional to the volume of the confidence ellipsoid around the parameter estimates. Moreover, Bayesian $\mathcal{D}$-efficient ($DB$) designs are obtained, instead of locally efficient designs, by minimizing the expectation of the $\mathcal{D}$-error over a prior distribution of the individual-specific coefficients.

At the start of the choice experiment there is no choice data available. Therefore a multivariate normal prior is assumed and the following criterion is minimized over all possible choice sets to select the first set in the design

$$DB = \int \det[\mathbf{I}_{BFIM}(\boldsymbol{\beta}_n, \mathbf{X}_n^1)]^{-1/p} \; f(\boldsymbol{\beta}_n) \; d\boldsymbol{\beta}_n, \tag{6}$$

with $f(\boldsymbol{\beta}_n) \equiv \phi(\boldsymbol{\beta}_n|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$.

Yet, when a respondent has completed some choice sets, say $s-1$, the prior information can be updated in a Bayesian way with the choice data available. The posterior distribution of the individual-specific coefficients given the choices of the $s-1$ previous choice sets then equals

$$f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}) = \frac{L(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, \mathbf{X}_n^{s-1}) \; \phi(\boldsymbol{\beta}_n|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)}{\int L(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, \mathbf{X}_n^{s-1}) \; \phi(\boldsymbol{\beta}_n|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0) \; d\boldsymbol{\beta}_n}. \tag{7}$$

Note that $f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}) \equiv f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, \mathbf{X}_n^{s-1}, \boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$, but the short form is applied for notational convenience.

This updated posterior is now used as the weighing distribution in the Bayesian $\mathcal{D}$-efficiency criterion to select the next best choice set for respondent $n$ by minimizing

$$DB = \int \det[\mathbf{I}_{BFIM}(\boldsymbol{\beta}_n, \mathbf{X}_n^s)]^{-1/p} \; f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}) \; d\boldsymbol{\beta}_n, \tag{8}$$

with $\mathbf{X}_n^s$ the design matrix including the $s-1$ perceived choice sets and the next $s$th choice set for respondent $n$. An additional set in an individualized choice experiment is thus obtained by minimizing the design's $\mathcal{D}$-error, weighted over the posterior distribution of the individual coefficients, hence "minimum posterior weighted $\mathcal{D}$-error". The process of alternately updating the posterior distribution of the coefficients with additional choice data and using this update to efficiently generate the next choice set can be continued until a specific amount of sets is administered.

### 2.2.2 Kullback-Leibler information design criteria

The Kullback-Leibler divergence, also denoted as the Kullback-Leibler distance or the Kullback-Leibler information, between two density functions $f$ and $g$ of a continuous variable $X$ is given by (Kullback and Leibler, 1951)

$$KL(f, g) \quad = \quad \int f(x) \; \log\frac{f(x)}{g(x)} \; dx. \tag{9}$$

The Kullback-Leibler divergence is commonly interpreted as a measure of distance between two densities.

In order to select the next best choice set for a specific respondent, one maximizes the distance between the current posterior of the coefficients (obtained with the choice data at hand) and the updated posterior one would obtain with the additional response information from the next choice set. Since a set in a choice experiment comprises multiple alternatives, we take the expectation over all possible choices and maximize the expected Kullback-Leibler distance between subsequent posteriors (Mulder and van der Linden, 2010).

Assume respondent $n$ has completed $s-1$ choice sets. The $s$th choice set in his/her design is then efficiently selected by maximizing

$$KLP = \sum_{k=1}^{K} \pi(y_{ksn}|\mathbf{y}_n^{s-1}) \; KL[f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}), f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, y_{ksn})] \tag{10}$$

over all possible sets, with $f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1})$ and $f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, y_{ksn})$ updated posteriors as in (7). Note that $y_{ksn}$ implies here that the $k$th alternative would be chosen in choice set $s$. The weights in (10) are defined as

$$\pi(y_{ksn}|\mathbf{y}_n^{s-1}) = \int p_{ksn}(\boldsymbol{\beta}_n)\ f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1})\ d\boldsymbol{\beta}_n \tag{11}$$

To select the first choice set in the design, when no choice data is available yet, the current posterior $f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1})$ in (10) and (11) is replaced by the normal prior $f(\boldsymbol{\beta}_n) \equiv \phi(\boldsymbol{\beta}_n|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$:

$$\sum_{k=1}^{K} \pi(y_{k1n})\ KL[f(\boldsymbol{\beta}_n), f(\boldsymbol{\beta}_n|y_{k1n})] \tag{12}$$

with

$$\pi(y_{k1n}) = \int p_{k1n}(\boldsymbol{\beta}_n)\ \phi(\boldsymbol{\beta}_n|\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)\ d\boldsymbol{\beta}_n. \tag{13}$$

Related to Kullback-Leibler divergence is mutual information, which for two continuous variables $X$ and $Y$ is defined as (Mulder and van der Linden, 2010; Weissman, 2007)

$$I_M(X,Y) = \int_Y \int_X f(x,y)\ \log \frac{f(x,y)}{f(x)f(y)}\ dxdy. \tag{14}$$

It is the Kullback-Leibler distance between the joint distribution of $X$ and $Y$ and their distribution in case of independence.

We follow Mulder and van der Linden (2010) and Wang and Chang (2011) and maximize the mutual information between the current posterior distribution of the individual coefficients and the posterior weighted choice probabilities for the alternatives in the next set, given the choice data of the previously administered sets. The criterion to be maximized over all possible sets is

$$MUI = \sum_{k=1}^{K} \left[ \int p_{ksn}(\boldsymbol{\beta}_n)\ \log\ p_{ksn}(\boldsymbol{\beta}_n)\ f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1})\ d\boldsymbol{\beta}_n - \pi(y_{ksn}|\mathbf{y}_n^{s-1})\ \log\ \pi(y_{ksn}|\mathbf{y}_n^{s-1}) \right]. \tag{15}$$

From (15) it can be concluded that also $MUI$, just as $KLP$, only requires the computation of posterior weighted choice probabilities for the alternatives in the next choice set.

The final design criterion used in this research is based on entropy. For a continuous variable $X$ and density $f(x)$, the entropy is defined by (Wang and Chang, 2011; Weissman, 2007)

$$H(X) = -\int f(x)\ \log\ f(x)\ dx \tag{16}$$

and is a measure of uncertainty. To efficiently select a subsequent choice set in an individualized choice experiment, we minimize expected posterior entropy (Wang and Chang, 2011) or equivalently maximize

$$ENT = \sum_{k=1}^{K} \pi(y_{ksn}|\mathbf{y}_n^{s-1}) \int f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, y_{ksn})\ \log\ f(\boldsymbol{\beta}_n|\mathbf{y}_n^{s-1}, y_{ksn})\ d\boldsymbol{\beta}_n. \tag{17}$$

| | Experimental setup | $\boldsymbol{\mu}$ | $\boldsymbol{\Sigma}$ |
|---|---|---|---|
| Scenario 1 | $3^3/2/15$ | (-0.5, 0, -0.5, 0, -0.5, 0) | $0.5 \times \mathbf{I}_6$ |
| Scenario 2 | $2 \times 3 \times 2 \times 3/3/15$ | (-0.5, -0.5, 0, -0.5, -0.5, 0) | $0.5 \times \mathbf{I}_6$ |
| Scenario 3 | $3 \times 2^4/2/15$ | (2.403, 1.648, 0.976, -0.613, -0.188, 2.008) | Appendix C |
| Scenario 4 | $3 \times 2 \times 3/3/15$ | (0.419, 0.700, 1.355, 1.638, 1.690) | Appendix C |

Table 1: Overview of the scenarios in the simulation study

# 3 Simulation study and results

In this section, we compare the criteria $DB$, $KLP$, $MUI$ and $ENT$ introduced above with respect to their efficiency and practicality in designing individualized choice experiments for the mixed logit choice model. We consider 4 scenarios that are summarized in Table 1. We assume 50 respondents in the experiments.

The third and the fourth scenario are based on empirical studies from respectively Carlsson et al. (2003) and Espino et al. (2008). In scenario 3 the profiles are defined by five attributes, the first with three levels, the remaining four with two, and choice sets include two alternatives. In the final setup there are three attributes with respectively 3, 2 and 3 levels and three alternatives in each set. In both cases, choice experiments with 15 sets are designed. Note that in agreement with the assumptions in Carlsson et al. (2003) and in Espino et al. (2008) the attributes are now dummy coded. The true values for $\boldsymbol{\Sigma}$ are given in Appendix C.

In all scenarios the initial prior $f(\boldsymbol{\beta}_n)$ used in the design criteria is assumed to be a multivariate normal distribution for which the prior values $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ equal the true values of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ in each scenario.

## 3.1 Estimation and prediction accuracy

We first discuss the accurateness of the estimates for the population parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ in the mixed logit choice model. To compare the estimation accuracy obtained with the different design criteria, we compute the root-mean-squared-errors $\mathrm{RMSE}_{\boldsymbol{\mu}}$ and $\mathrm{RMSE}_{\boldsymbol{\Sigma}}$ which measure the estimation error for respectively $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$. They are given by

$$\mathrm{RMSE}_{\boldsymbol{\mu}} = \sqrt{\frac{(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu})'(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu})}{p}}, \tag{18}$$

with $\hat{\boldsymbol{\mu}}$ and $\boldsymbol{\mu}$ respectively the estimates and the true values of the mean effects and $p$ the number of coefficients in the model and

$$\mathrm{RMSE}_{\boldsymbol{\Sigma}} = \sqrt{\frac{(\hat{\boldsymbol{\sigma}} - \boldsymbol{\sigma})'(\hat{\boldsymbol{\sigma}} - \boldsymbol{\sigma})}{p_{\boldsymbol{\Sigma}}}}, \tag{19}$$

with $\boldsymbol{\sigma}$ stacking all the unique elements from $\boldsymbol{\Sigma}$, $\hat{\boldsymbol{\sigma}}$ the estimates and $p_{\boldsymbol{\Sigma}}$ equal to $p(p+1)/2$, the number of elements in $\boldsymbol{\sigma}$.

Note that for each design algorithm and for each scenario, the generation of the choice designs and the estimation of the mixed logit choice model was repeated 100 times. The mean $\mathrm{RMSE}_{\boldsymbol{\mu}}$ and $\mathrm{RMSE}_{\boldsymbol{\Sigma}}$ values are given in Figure 1 for each scenario and all four design criteria. In the first two and the fourth scenario, no significant differences in $\mathrm{RMSE}_{\boldsymbol{\mu}}$ and $\mathrm{RMSE}_{\boldsymbol{\Sigma}}$ are

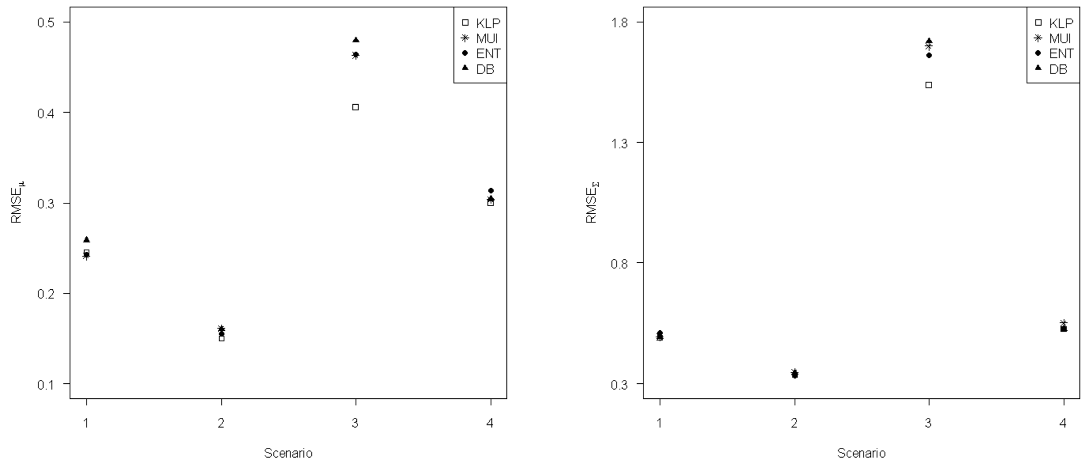


Figure 1: Mean $\text{RMSE}_{\boldsymbol{\mu}}$ and $\text{RMSE}_{\boldsymbol{\Sigma}}$ values obtained with $KLP$, $MUI$, $ENT$ and $DB$ for the different scenarios

observed. The population parameters in the model are estimated equally accurate with all four design criteria. In scenario 3 however, $KLP$ outperforms the other methods as its $\text{RMSE}_{\boldsymbol{\mu}}$ and $\text{RMSE}_{\boldsymbol{\Sigma}}$ are significantly smaller than the corresponding estimation errors obtained with $MUI$, $ENT$ and $DB$.

Besides modeling aggregate choice behavior, it might also be of interest to have a view on individual preferences and to obtain good estimates for the coefficients $\boldsymbol{\beta}_n$ in the mixed logit choice model. Therefore, in addition to $\text{RMSE}_{\boldsymbol{\mu}}$ and $\text{RMSE}_{\boldsymbol{\Sigma}}$, the root-mean-squared-error $\text{RMSE}_{\boldsymbol{\beta}}$ is also compared between the design criteria:

$$\text{RMSE}_{\boldsymbol{\beta}} = \sqrt{\frac{1}{N}\sum_{n=1}^{N}\frac{(\hat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}_n)'(\hat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}_n)}{p}}, \tag{20}$$

with $\hat{\boldsymbol{\beta}}_n$ and $\boldsymbol{\beta}_n$ respectively the estimates and the true values for the coefficients of person $n$ and $N$ the number of respondents. Figure 2 shows the mean values of the $\text{RMSE}_{\boldsymbol{\beta}}$ over the 100 simulations for each design criterion and each scenario.

With respect to the individual coefficients, $KLP$ again outperforms the remaining methods in scenario 3 as its $\text{RMSE}_{\boldsymbol{\beta}}$ value is significantly smaller than the estimation errors of $MUI$, $ENT$ and $DB$. For all other scenarios, no clear differences in estimation error are observed.

## 3.2 Computation time

The main asset of the Kullback-Leibler design criteria is that they are much easier to compute than the $DB$ criterion. Although computing $KLP$, $MUI$ and $ENT$ also requires the weighing of choice probabilities over sequentially updated posteriors, the criteria do not involve the time consuming computation of the determinant of the Fisher information matrix, incorporating all sets in the choice experiment. Consequently, selecting the next best set in an individualized choice experiment is much faster with $KLP$, $MUI$ and $ENT$ than with $DB$.

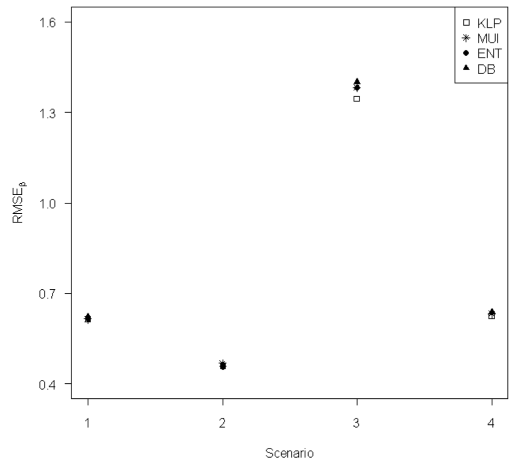


Figure 2: Mean RMSE$_{\boldsymbol{\beta}}$ values obtained with $KLP$, $MUI$, $ENT$ and $DB$ for the different scenarios

| | Scenario 1 | Scenario 2 | Scenario 3 | Scenario 4 |
|---|---|---|---|---|
| $KLP$ | 0.074 | 1.726 | 0.207 | 0.219 |
| $MUI$ | 0.082 | 1.773 | 0.215 | 0.223 |
| $ENT$ | 0.090 | 1.972 | 0.242 | 0.246 |
| $DB$ | 1.789 | 35.689 | 5.207 | 3.855 |

Table 2: Average computation time (seconds) for selecting one additional choice set with $KLP$, $MUI$, $ENT$ and $DB$

To demonstrate this, Table 2 displays the average computation time (in seconds) to sequentially generate one additional set in a choice design using respectively $KLP$, $MUI$, $ENT$ and $DB$ as selection rule. The decrease in computation time from using the Kullback-Leibler design criteria instead of $DB$ is impressive.

# 4 Conclusion

Individualized choice experiments are designed with respect to the individual preferences of a specific respondent, sequentially taking previous choices into account to select the next choice set. With individual-specific coefficients in the model, designing choice experiments at an individual level is more efficient than using an aggregate design approach. Three new design criteria, alternative to $\mathcal{D}$-efficiency, are presented to speed up the construction of the individualized designs.

In a simulation study the Kullback-Leibler criteria are compared with $\mathcal{D}$-efficiency under various experimental settings. The conclusion is clear: the design efficiency of the four criteria to estimate the mixed logit choice model is equivalent. As the Kullback-Leibler based designs are much faster to compute than those based on the $\mathcal{D}$-efficiency criterion, these are to be preferred.

# A Matrices $\Sigma$ in scenario 3 and 4

$$\mathbf{\Sigma}_3 = \begin{pmatrix} 6.605 & 6.784 & 3.299 & 2.059 & 2.246 & 1.855 \\ 6.784 & 8.231 & 4.838 & 3.018 & 3.290 & 2.721 \\ 3.299 & 4.838 & 7.007 & -0.547 & 2.424 & -0.186 \\ 2.059 & 3.018 & -0.547 & 5.392 & 2.339 & 2.344 \\ 2.246 & 3.290 & 2.424 & 2.339 & 3.964 & 1.663 \\ 1.855 & 2.721 & -0.186 & 2.344 & 1.663 & 9.358 \end{pmatrix}$$

$$\mathbf{\Sigma}_4 = \begin{pmatrix} 0.047 & 0 & 0 & 0 & 0 \\ 0 & 0.906 & 0 & 0 & 0 \\ 0 & 0 & 2.632 & 0 & 0 \\ 0 & 0 & 0 & 0.568 & 0 \\ 0 & 0 & 0 & 0 & 1.107 \end{pmatrix}$$

# Acknowledgements

Research funded by ZKC1090 / DBOF/08/014 - DBOF project of the KU Leuven

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