

# **Discrete Decisions with Model Validation** using Probabilistic Inversion

PROEFSCHRIFT

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*Rabin Neslo*







# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Motivation and Outline . . . . .	1
1.2	Definitions and Formalism . . . . .	6
1.2.1	Paired Comparisons . . . . .	9
1.2.2	Existence of a Random Utility function . . . . .	10
1.3	Deriving a Random Utility Function using Probabilistic Inversion . . . . .	13
1.3.1	From Stakeholders' Preference to Random Utility . . . . .	14
1.4	Multi Criteria Decision Making and Probabilistic Inversion . . . . .	20
1.5	Model Validation . . . . .	21
<b>2</b>	<b>Independence of Irrelevant Alternatives</b>	<b>23</b>
2.1	Introduction . . . . .	23
2.2	IIA . . . . .	24
2.3	Implications of IIA . . . . .	26
2.3.1	From Preferences to Shares . . . . .	26
2.3.2	Scenario One . . . . .	28
2.3.3	Scenario Two . . . . .	28
2.3.4	Scenario Three . . . . .	30
2.3.5	Scenario Four . . . . .	31
2.4	Conclusion . . . . .	33
<b>3</b>	<b>Minimum Information and Independence in Discrete Choice</b>	<b>35</b>
3.1	Introduction . . . . .	35
3.2	Minimal Relative Information Solution of a Uniform Distribution Without Independence . . . . .	36
3.2.1	Two Choice Alternatives . . . . .	37

3.2.2	<i>N</i> Choice Alternatives . . . . .	42
3.3	Minimal Relative Information Solution with a Standard Uniform Distribution Assuming Independence . . . . .	44
3.3.1	Two Choice Alternatives . . . . .	44
3.3.2	<i>N</i> Choice Alternatives . . . . .	45
3.3.3	Results Uniform distribution with Two Choice Alternatives . . . . .	47
3.3.4	Results Uniform distribution with Three Choice Alternatives . . . . .	49
3.4	Normal distribution : Probit model . . . . .	50
3.4.1	Minimal Information Solution for Two Alternatives . . . . .	50
3.4.2	Minimal Information Solution for Three Alternatives . . . . .	54
3.4.3	Results Normal distribution with Three Choice Alternatives . . . . .	57
3.5	Appendix . . . . .	59
<b>4</b>	<b>Application to Prioritizing Marine Ecosystem Vulnerabilities</b>	<b>69</b>
4.1	Background . . . . .	69
4.2	The Model . . . . .	70
4.3	Results and Validation . . . . .	71
4.3.1	Model Adequacy . . . . .	71
4.3.2	Criteria Weights . . . . .	73
4.3.3	Scenario Scores . . . . .	81
4.4	Conclusion . . . . .	84
<b>5</b>	<b>Application to Strategic Risk Planning in Public Health</b>	<b>85</b>
5.1	Background . . . . .	85
5.2	Steps for employing the model . . . . .	88
5.2.1	Step 1 - criteria employed to characterize scenarios . . . . .	88
5.2.2	Step 2 - Scenarios: health states . . . . .	88
5.2.3	Step 3 - Survey's layout . . . . .	90
5.3	Step 4 - The Model . . . . .	93
5.4	Step 5 - Model adequacy and Results . . . . .	94
5.4.1	Expert consistency . . . . .	94
5.4.2	Random preference orderings . . . . .	95
5.4.3	Savage rationality . . . . .	96
5.4.4	Multi Criteria Decision Making (MCDM) . . . . .	96
5.4.5	Criteria Weights . . . . .	98
5.4.6	Health State Scores . . . . .	100
5.4.7	Out-of-sample validation . . . . .	102
5.5	Conclusion . . . . .	106

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<b>6</b>	<b>Application to The Risk Assessment of Nano-Enabled Food Products</b>	<b>107</b>
6.1	Background . . . . .	107
6.2	Steps for employing the model . . . . .	109
6.2.1	Step 1 - criteria employed to characterize the food products	109
6.2.2	Step 2 - scenarios: nanotechnology enabled food products .	109
6.2.3	Step 3 - Scoring matrix . . . . .	110
6.2.4	Step 4 - identifying and recruiting the experts . . . . .	111
6.2.5	Step 5 - survey format . . . . .	111
6.2.6	Step 6 - the model . . . . .	112
6.3	Results and Validation . . . . .	112
6.3.1	Model Adequacy . . . . .	112
6.3.2	Criteria Weights . . . . .	118
6.3.3	Safety Scores . . . . .	125
6.3.4	Fresh Expert / Alternative Validation . . . . .	125
6.4	Conclusions . . . . .	131
<b>7</b>	<b>Conclusion</b>	<b>133</b>
7.1	Model Validation . . . . .	134
7.1.1	Consistency with Discrete Choice Data . . . . .	134
7.1.2	Consistency with Savage Rationality . . . . .	134
7.1.3	In Sample Validation . . . . .	134
7.1.4	Out Sample Validation . . . . .	135
7.1.5	Fresh Alternative/Stakeholder Validation . . . . .	135
7.2	Recommendations and Future Work . . . . .	135
<b>A</b>	<b>Software Used</b>	<b>137</b>
A.1	Background . . . . .	137
A.2	User Manual . . . . .	138
	<b>References</b>	<b>157</b>
	<b>Summary</b>	<b>165</b>
	<b>Samenvatting</b>	<b>167</b>
	<b>Curriculum Vitae</b>	<b>169</b>



# Introduction

## 1.1 Motivation and Outline

Savage [82] formulated axioms for rational preference of an individual, and showed that the preferences of a rational agent can be represented as expected utility, where the individual's subjective probability over possible states of the world is unique and the utility function over consequences is affine unique. The representation of a preference relation by a utility function implies that an individual assigns higher expected utility to choice alternative  $a$  than to alternative  $b$ , if and only if the individual prefers, selects or orders an alternative  $a$  above  $b$ .

Whereas the theory of subjective probability has flourished; it is fair to say that the modeling of utility has lagged behind. Without reviewing the activity in this area, suffice to say that, in our opinion, there are two major causes for this. First, modeling techniques like multi attribute utility theory (MAUT), multi criteria decision making (MCDM), etc. focus on capturing "the" utility function over choice alternatives. If an individual's utility function conformed to additional (rather severe) constraints<sup>1</sup>, such a representation might be possible at an individual level. However, there is no reason to believe that "a" utility function exists for groups of individuals; the search for such is a fool's errand. Based on the theory of rational decision, the proper goal of utility modeling should be to capture the distribution over utility functions characterizing a group. Second, and perhaps not wholly unrelated, there has been a near total absence of attempts to validate the utility models produced by these various methods. As such, the field of applied utility theory remains parochial. There is a wealth of literature demonstrating that stakeholders often violate the axioms of rational preference. This does not threaten the normative status of the theory any more than the pre-

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<sup>1</sup>A couple of these constraints are *Additive Utility Independence*, *Utility Independence*, *Mutually Utility Independent*, see Keeney and Raiffa [36], French [27]

valence of invalid inferences imperils logic. However, it does lend urgency to the issue of validation.

The prospects for utility theory are brighter within the literature of discrete choice and random utility theory. Thurstone [91] pioneered this field with his celebrated law of comparative judgment. Assuming that utilities are normally distributed over a population of stakeholders, he fits the parameters of this distribution, under various correlation assumptions, using discrete choice data from pairwise comparisons. Luce [55] later derived a different random utility model called the Logit model [6], [57] under one of the consequences of Luce's choice axioms namely the *Independence of Irrelevant Alternatives* (IIA). McFadden [60] also derived the Logit model under the random utility maximization principle. The Logit models assume that the error terms are generalized extreme value (GEV) distributed with mean zero and some constrained covariance matrix. Unhappy with the IIA assumption, McFadden and Train [64] picked up the thread of random utility maximization and extended the standard version of the Logit and Probit model, to deal with the limitations they pose. Whereas goodness of fit tests have been developed for many random utility models, true out-of-sample validation is not part of standard operating procedure.

The problem of inferring a distribution over utility functions from discrete choice data is a problem of probabilistic inversion. Theory tells us that each (rational) stakeholder has a utility function; if we knew these utility functions for a group of stakeholders we could predict the distribution of responses in discrete choice situations. We observe the distribution of responses and wish to infer the distribution over utility functions. Even more, we wish to model these utility functions as functions of physical attributes of the choice alternatives, and we wish to infer rather than impose dependence relations between utilities. This program is quite feasible, albeit that the techniques for solving probabilistic inversion problems are new to this field. A few applications are in press, or have been published [71], [10], [90], [49]. This approach also allows us to capture a distribution over utility functions non-strict preferences from the stakeholders, see chapter 2. It also allows us to perform true out-of-sample validation.

To motivate the approach we consider the health state valuation problem [72]. Currently, health states are described and valued using EQ-5D<sup>2</sup>. EQ-5D is a standardized measure of health states developed by the EuroQol Group in order to provide a simple, generic measure of health for clinical and economic appraisal. Each health state is characterized by five criteria (mobility, self-care, usual activities, pain-discomfort, and anxiety-depression) which are measurable quantities that increase in a monotonic scale taking values one, two, three. An extended version (i.e. EQ-5D+C; see Table 5.2.1 in the Appendix) of the system was introduced by Stouthard et al. [87], which we use. These different health states are possible outcomes of therapeutic procedures, and their valuation is critical in deciding which procedures to support and supply.

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<sup>2</sup>Further information can be found in <http://www.euroqol.org>

With 6 criteria taking 3 possible values, there are  $3^6 = 729$  possible health states. The most direct approach would be to ask a group of stakeholders randomly chosen from the target population, to state their utility values for each health state. To estimate the distribution of utility functions, each stakeholder should apply a standardized utility scale with common zero and unit. The assessment burden for the stakeholders would be forbidding.

Although the distribution over utilities of these health states is the immediate goal; we want also to model the utility of health states in terms of the attribute scores. Existing approaches will often ask stakeholders to value the *attributes* and the *attribute scores*. This however is problematic for a number of reasons: (1) Whereas we choose health states in choosing a therapeutic procedure, we don't choose attributes as such. (2) The value attached to one attribute (eg "mobility") will depend on the whole set of attributes, as we must know what exactly falls under "usual activities" and "self care" to avoid double counting. Of course, valuing mobility score 3 versus mobility score 2 assumes that these values are unaffected by the values of other attributes. (3) It is unclear how the resulting distribution over health state utilities would be validated.

By adopting a simple model of the utility of a health state in terms of its attribute scores, we can simultaneously lighten the assessment burden and enable validation of the model. The score (utility) of health state  $i$  for subject  $s$  is modeled as:

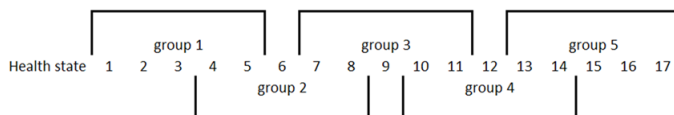
$$u_s(a_i) = \sum_{j=1}^6 \omega_{s,j} \times c_{i,j}; \sum_{j=1}^6 \omega_{s,j} = 1; \omega_{s,j} > 0, \quad (1.1.1)$$

where  $\omega_{s,j}$  is the weight for attribute  $j$  for subject  $s$  and  $c_{i,j}$  is the score of health state  $i$  on attribute  $j$ . If this model is adequate, the distribution of utility functions over the set of stakeholders may be captured as a distribution over attribute weights  $(\omega_1, \dots, \omega_6)$ . If the model is not adequate, a better model must be sought. Instead of asking each stakeholder for his/her weight vector, we will ask them to rank order subsets of the 729 health states, and look for a distribution over weight vectors which recovers the pattern of rankings. Given a single ranking of a set of health states, we could in principle recover the set of weight vectors which would yield this ranking under model (1.1.1). For a set of rankings we could take the union of the corresponding sets of weight vectors. The uniform distribution over this set could be taken as our distribution over utility functions. Although this is a feasible approach, it is not the one we adopt. To understand why, we must discuss the discrete choice format.

729 health states is much too many for stakeholders to rank order. A *discrete choice format* is needed render the assessment burden bearable. Best practice suggests that stakeholders can rank at most 7 items at a time. The most popular discrete choice format is simple pairwise comparisons: subjects are presented with all pairs of choice alternatives and asked to choose one of the two offered. This is obviously infeasible for 729 alternatives, as there are 265,356 pairs. An

economical discrete choice format is acceptable if it enables validation of the model on which it is based. For the present study we selected 17 non-dominated health states<sup>3</sup>. These 17 health states are broken into 5 overlapping groups of 5, where stakeholders then rank the health states in each group. The overlap structure is shown in Figure (1.1.1)

Figure 1.1.1: *Overlap structure*



Some pairs of states occur in two groups of 5, which enables us to screen stakeholders for consistency. A stakeholder who ranks health state  $i$  above health state  $j$  in group  $k$  is called inconsistent if he ranks health state  $j$  above health state  $i$  in group  $k + 1$ . With this discrete choice format we gather data which we then use to infer a distribution over the utility values. One of the goals in choosing a discrete choice format is to enable the analyst to identify inconsistent respondents. Removing inconsistent experts can produce better results. Depending on the format, it may be unrealistic to expect perfect consistency. In pairwise comparisons, for example, it is usually sufficient that the number of inconsistencies (circular triads) is small enough to reject the hypothesis that a subject is choosing his/her preferences at random. Thus a solution strategy for finding a distribution over utility vectors must be able to deal with inconsistency: even if there is no distribution over utility vectors which *exactly* reproduces the stakeholders' responses, it may be possible to minimize the lack of fit and thus arrive at a reasonably well validated model. Choosing a discrete choice format mixes science and craft, and as this approach to utility quantification is relatively recent, the craft is still evolving.

The necessity of dealing with inconsistencies drives our choice of solution technique. If the problem is feasible, the solution algorithm should converge to a unique solution, if the problem is not feasible, then it should converge to a unique distribution which minimizes lack of fit in some appropriate sense. We proceed as follows. For each group we define a square *preference ranking matrix* whose  $i, j$ -th entry gives the proportion of stakeholders who ranked health state  $i$  in the  $j$ -th position, in that group. The task is to find a distribution over the weights that reproduce the preference ranking matrices. Initially a diffuse distribution is chosen over the weights from which a large sample is drawn. For each sample weight vector we can compute how a stakeholder with that weight vector and model (1.1.1) would rank the health states in each 5-group. The entire

<sup>3</sup>The attribute scores increase in severity: pain score 3 is worse than pain score 1, etc. Health state  $i$  dominates health state  $j$  if  $i$ 's score on each criteria is greater than  $j$ 's.



sample will lead to 5 preference ranking matrices which will not agree with those from our stakeholder data. Iterative re-weighting schemes like Iterative Proportional Fitting (IPF; see section 1.3.1) will then assign differential weights to each of the original samples such that if we resample this sample distribution using these weights, the resulting preference ranking matrices agree - to the extent possible - possible - with those of the stakeholders. If the problem is feasible, IPF converges quickly and gives the unique solution which is minimally informative with respect to the initial sample distribution. In case the problem is infeasible, other techniques like PARFUM (see section 1.3.1) guarantee a solution that is the least infeasible in an appropriate sense.

Having obtained a solution using the solution techniques, we validate the solution by splitting the entries of the five preference ranking matrices into a test set and a validation set. The model is initialized on the test and used to predict values in the validation set. Procedures of this kind are termed out-of-sample validation. In the following sections of this chapter we give more detailed information about the discrete choice format, solution techniques and out-of-sample validation.

The outline of the thesis is given as follows. In chapter 1 we introduce the concept of stakeholders' preferences and random utility. We propose definitions and formalism which extend the formulations of discrete choice. Together with these formalisms and *Probabilistic Inversion* (PI) we have created alternative techniques for deriving a distribution over utility functions. These PI techniques allow us to validate discrete choice models.

In chapter 2 we examine the *Independence of Irrelevant Alternatives* principle and its consequences. The definitions and formalism from chapter 1 enable us to resolve the the problems that occur when using a distribution over the utility functions that satisfies the *Independence of Irrelevant Alternatives*. It has been shown by Marschak [57] that *Independence of Irrelevant Alternatives* imposes additional constraints over stakeholders' preferences for the existence of a distribution over utility functions.

In chapter 3 we formulate a discrete choice problem as an optimization problem. We assume a given starting or prior distribution over the utility functions. Given this starting distribution we seek a posterior distribution over utility functions that satisfies stakeholders' preferences while being as close as possible to the starting distribution in terms of the Kullback-Leibler measure. It follows that the distribution obtained with PI techniques discussed in chapter 1 is equivalent with the distribution that follows from the optimization problem. In many cases PI techniques will find a distribution over utility functions when the optimization problem becomes intractable. We also study the implications of different starting distributions with and without independence.

The most recent application is given in chapter 6. Our techniques for MCDM are applied to find a basic screening model for the safety of nanotechnology enabled food products, see Flari et al. [24]. Although the benefits of using nanoparticles in food products are potentially many, i.e. fewer quantities needed, the risks have yet to be determined and also assessed adequately. Doing a case by case

study is not possible, because there is few to no data available about the safety of nanotechnology enabled food products. With stakeholders' preferences and PI we capture knowledge about the safety of such products and use the preferences to fit a screening model based on a set on 10 criteria.

The second application is given in 5. The idea of modeling health states as a random utility model with underlying physical attributes is not new [81]. Whereas these studies attempt to extract valuations on criteria (criteria weights), this study aimed to improve an existing model EQ-5D+C for valuing health states using stakeholders' preferences on health states directly. The idea is that applying stakeholders preferences to the model will lead to more transparent and defensible assessment of the MCDM model.

The application in chapter 4 concerns the prioritization of ecosystem in the California coastal area [71, 90]. The criteria used in this MCDM model intend to capture the vulnerability of the ecosystems. Weights fitted to the model using stakeholders' preferences on 30 ecosystems are used to determine the threat potential of all the remaining ecosystems.

## 1.2 Definitions and Formalism

As noted already by Savage [82] simple binomial or multinomial discrete choice data (paired comparisons, multiple choices) do not enable us to distinguish strict preference from equivalence in preference. That is, if a subject presented with a choice between alternatives  $a$  and  $b$  chooses  $a$ , we may only conclude that for him/her,  $a$  is at least as good as  $b$ . While this might not be severe in modeling the preferences of one individual, for populations of stakeholders, such ambiguity can cause problems. Thus if 50% of stakeholders preferred a red bus to a blue bus, and 50% preferred the blue to red bus, this might either mean that everyone had strict preferences evenly divided over the population, or alternatively it might mean that everyone in the population was indifferent to the buses' color, and was choosing one color at random. Failure to distinguish these cases can cause problems in modeling the preferences of the population see chapter 2. These issues are important and have dominated a good deal of the discrete choice literature. The tools that we develop for deriving a distribution over utility functions, given a distribution of responses to a discrete choice problem apply equally well for strict and non-strict preference. However, allowing for equivalence in preference considerably complicates the notation, as can be inferred from Definition 2.

Discrete choice or random utility models describe and analyze the preferences of a group of stakeholders  $S$  for set of choice alternatives. We denote this non-empty set of choice alternatives by  $\mathcal{A} = \{a_1, \dots, a_N\}$ . The preferences of each stakeholder are denoted in the customary way as  $a_i \succeq a_j$ . If necessary to distinguish  $s \in S$ , we will write  $\succeq_s$ .

Savage's [82] theory of rational decision ensures that the preferences of a single rational stakeholder can be expressed in terms of expected utility. Each

$s \in \mathcal{S}$  may be assigned a utility function over choice alternatives that is unique up to a positive affine transformation. If  $u : \mathcal{A} \rightarrow \mathbb{R}$  is a utility function for a given stakeholder, then  $cu + d, c > 0, d \in \mathbb{R}$ , is also a utility function for this stakeholder. We will assume that our set of stakeholders have utility functions which can be assigned the same unit. This means that there are two consequences, say  $g$  and  $b$ , not necessarily belonging to the choice set  $\mathcal{A}$ , such that all stakeholders agree that  $g$  is strictly preferred to  $b$ . Each stakeholder would then choose respectively  $g$  and  $b$  as the unit and zero of his utility scale. We call such a set of stakeholders *orientable*. Since the number of choice alternatives is always finite, there is no restriction in assuming that the utilities of an orientable set of rational stakeholders over  $\mathcal{A}$  may be represented as standardized  $\mathcal{A}$ -vectors taking values in  $[0, 1]$ , that is, as elements of  $[0, 1]^{\mathcal{A}}$ .

**Definition 1.**  $\mathcal{D}$  is called a discrete choice problem on  $\mathcal{A}$  if

1.  $\mathcal{A} = a_1, \dots, a_N$  is a finite non-empty set of  $N$  choice alternatives
2.  $\mathcal{D} = \{D_1, \dots, D_K | D_i \subseteq \mathcal{A}, D_i \neq \emptyset, i = 1, \dots, K\}$

A familiar type of a discrete choice problem is paired comparisons. Choice alternatives are presented in  $\binom{N}{2}$  pairs from which stakeholders pick their (strictly) preferred alternative.

The response of a stakeholder to a discrete choice problem may take many forms. For example, (s)he may choose a unique preferred alternative from each set  $D_k \in \mathcal{D}$  (strict choice) or a set of non-dominated alternatives in  $D_k \in \mathcal{D}$  (non-dominated choice), or (s)he may order the elements of  $D_k \in \mathcal{D}$ , such that the response is a permutation  $\pi \in D_k!$  (strict preference order), or (s)he may produce an ordered partition of elements  $D_k$  where the alternatives in each element of the partition are equivalent (non-dominated preference order). These are captured in

**Definition 2.** • A strict choice response from  $\mathcal{S}, r = (r_1, \dots, r_K)$  to discrete choice problem  $\mathcal{D}$  is a set of mappings  $r_k : \mathcal{S} \rightarrow D_k, k = 1 \dots K$ .

- A non-dominated choice response from  $\mathcal{S}, r = (r_1, \dots, r_K)$  to discrete choice problem  $\mathcal{D}$  is a set of mappings  $r_k : \mathcal{S} \rightarrow 2_+^{D_k}$ , with  $2_+^{D_k} = 2^{D_k} \setminus \emptyset, k = 1 \dots K$ .
- A strict preference order response from  $\mathcal{S}, r = (r_1, \dots, r_K)$  to discrete choice problem  $\mathcal{D}$  is a set of mappings  $r_k : \mathcal{S} \rightarrow D_k!$  where  $D_k!$  is the set of permutations of  $D_k, k = 1 \dots K$ .
- A non-dominated preference order response from  $\mathcal{S}, r = (r_1, \dots, r_K)$  to discrete choice problem  $\mathcal{D}$  is a set of mappings  $r_k : \mathcal{S} \rightarrow \Pi_k$  where  $\Pi_k$  is the set of ordered partitions of  $D_k, k = 1 \dots K$ .

The set of all possible responses to  $\mathcal{D}$  for all  $s \in \mathcal{S}$  will be denoted by  $r_{\mathcal{D}}$ . Many other response forms are conceivable, but the above are the most straightforward. Note the difference between strict and non dominated choice. In the standard versions of random utility theory, when a stakeholder chooses element  $a_i$  from a set  $\{a_1, \dots, a_N\}$ , this is interpreted to mean that  $a_i$  is at least as good as the other elements.

**Definition 3.** A probability mass function  $P$  over  $\mathcal{S}$  induces a probability mass function  $Q$  over  $r_{\mathcal{D}}$  as  $Q(r_k) = P(s \in \mathcal{S} | r_k(s) = r_k)$

The probability mass function  $P$  over  $\mathcal{S}$  will usually be the counting measure. The probability of  $r_k$  is then:

$$Q(r_k) = \frac{\sum_{s \in \mathcal{S}} 1_{r_k(s)=r_k}}{|\mathcal{S}|}. \quad (1.2.1)$$

**Definition 4.** Let  $\mathcal{S}$  be an orientable finite set of rational stakeholders, whose utilities  $u_s(a_i)$  for  $a_i \in \mathcal{A}, s \in \mathcal{S}$  take values in  $[0, 1]$ ; let  $\Omega = [0, 1]^N$ .  $\mathcal{P}$  over  $2^\Omega$  is the probability mass function induced by  $P$  over  $\mathcal{S}$  if  $\mathcal{P}\{B \in 2^\Omega\} = P\{s \in \mathcal{S} | (u_s(1), \dots, u_s(N)) \in B\}$ . The utility  $u_i$  of  $a_i$  is a random variable whose distribution function is given as  $\mathcal{P}\{u_i \leq v\} = P\{s \in \mathcal{S} | u_s(i) \leq v\}, v \in [0, 1]$ .

Note that  $\mathcal{P}$  depends on  $\mathcal{S}$ , although we suppress this fact in the notation. Definition 4 simply says that an orientable set of rational stakeholders whose utilities are constrained to the  $[0, 1]$  interval induces a probability mass function on the set of utility vectors.

**Definition 5.**  $B_i$  is a cylinder set of  $\Omega$  if  $B_i = [0, 1] \times [0, 1] \times \dots \times B_i^* \times \dots \times [0, 1]$ , with  $B_i^* \subset [0, 1]$

**Definition 6.** The utilities for  $a_i, a_j$  are independent under  $\mathcal{P}$  if for all  $B_i, B_j$ ,

$$\begin{aligned} \mathcal{P}(B_i \cap B_j) &= P(s \in \mathcal{S} | u_s(a_i) \in B_i^* \cap u_s(a_j) \in B_j^*) \\ &= \mathcal{P}(B_i) \mathcal{P}(B_j) \end{aligned}$$

It follows that a population of stakeholders induces both a distribution over responses as well as distribution over utility values (see figure 1.2.1). The responses are indirectly induced from the utility values, because each stakeholder is associated with a utility vector  $u_s(\mathcal{A}) = (u_s(a_1), \dots, u_s(a_N))$ . If we knew the utility function of a stakeholder  $s \in \mathcal{S}$ , then we could obviously predict with certainty how  $s$  would respond to a discrete choice problem. Equivalently, if we are given a vector of utility values over the choice alternatives, we can uniquely determine how a stakeholder with that utility would respond in any discrete choice problem.

Our problem is to infer a distribution over (standardized) utility functions given a set of responses from stakeholder population  $\mathcal{S}$  (see figure 1.2.2). With the distribution over the utility values we will be able to compute measures like the means, standard deviations, and correlation coefficients of the utility values.

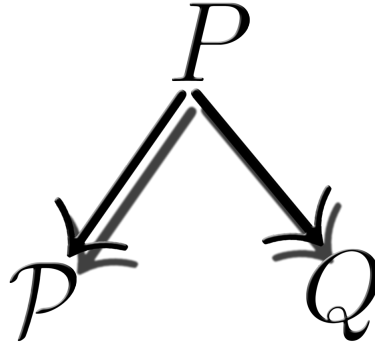


Figure 1.2.1:  $P$  inducing  $\mathcal{P}$  and  $Q$

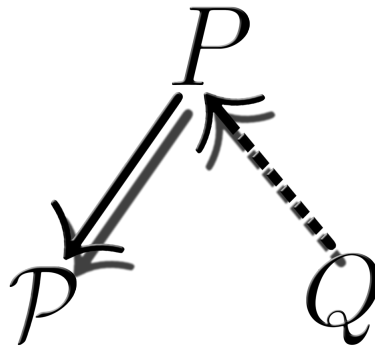


Figure 1.2.2: Inferring  $\mathcal{P}$  from  $Q$  via  $P$

### 1.2.1 Paired Comparisons

A simple paired comparison problem will illustrate the definitions. The choice set  $\mathcal{A} = \{a_1, \dots, a_N\}$  consists of a finite set of alternatives; stakeholders are presented with each pair of alternatives, and asked to choose their strictly preferred alternative from each pair.

$\mathcal{D} = \{\{a_1, a_2\}, \{a_1, a_3\}, \dots, \{a_{N-1}, a_N\}\}$ , where each pair occurs exactly once.

Each stakeholder chooses exactly one element from each pair. Let  $P$  be the counting distribution over  $\mathcal{S} : P(s) = \frac{1}{|\mathcal{S}|}$ .

For each pair  $D_{ij} = \{a_i, a_j\}$  the induced distribution over the response  $\{a_i\}$  may be represented as

$$\begin{aligned} Q(r_{ij} = \{a_i\}) &= P(s \in \mathcal{S} | r_{ij}(s) = a_i) \\ &= P(s \in \mathcal{S} | u_s(a_i) > u_s(a_j)) \\ &= \mathcal{P}(u(a_i) > u(a_j)) \end{aligned}$$

## 1.2.2 Existence of a Random Utility function

It might not always be possible to derive a random utility function over a set of choice alternatives given a distribution over the responses. For three choice alternatives and simple paired comparisons there are necessary and sufficient conditions for the existence of a random utility function[57]. Let the distribution over the responses be the counting distribution defined in the previous subsection. Then the probability of strict response  $a_i$  to  $D_{ij} = \{a_i, a_j\}$  is given by

$$\begin{aligned} Q(r_{ij} = a_i) &= P(s \in \mathcal{S} | r_{ij}(s) = a_i) \\ &= \frac{1}{|\mathcal{S}|} \sum_{s=1}^{|\mathcal{S}|} 1_{\{r_{ij}(s)=a_i\}} \\ &= \alpha_{ij}, \end{aligned} \tag{1.2.2}$$

with  $0 \leq \alpha_{ij} \leq 1$ . Marschak [57] gave necessary and sufficient conditions for the existence of a random utility function for three choice alternatives:

**Proposition 1.2.1.** *For paired comparison data with strict preferences on three choice alternatives  $a_1, a_2, a_3$ , with  $\alpha_{ij} = Q(a_i \succ a_j)$ , there exists a joint distribution  $\mathcal{P}$  over  $u \in [0, 1]^3$  such that  $\mathcal{P}\{u_i > u_j\} = \alpha_{ij}$ ,  $i, j = 1..3; i \neq j$  if and only if*

$$1 \leq \alpha_{12} + \alpha_{23} + \alpha_{31} \leq 2.$$

Any cyclic permutation of the indices  $(1, 2, 3)$  yields the same inequalities. The other permutations are cycles of  $(1, 3, 2)$ , and using  $p_{ij} = 1 - p_{ji}$  it is easy to check that these satisfy a similar inequality. To prove proposition 1.2.1 Marschak [57] assumed that any paired comparison can be written as a combination of preference orders e.g. permutations from the set  $\mathcal{A} = \{a_1, a_2, a_3\}$ . Inequality 1.2.1 must be relaxed to obtain necessary and sufficient conditions for non-strict preferences in paired comparisons of three alternatives. Before doing that we need to stipulate the following for the paired comparisons.

**Definition 1.2.2.** *If  $\succ$  represents strict preference, and  $\sim$  represents equivalence in preference, then a pairwise preference scheme is transitive for non-strict preference:*

- if  $a_i \succ a_j$  and  $a_j \succ a_k$ , then  $a_i \succ a_k$
- if  $a_i \succ a_j$  and  $a_j \sim a_k$ , then  $a_i \succ a_k$
- if  $a_i \sim a_j$  and  $a_j \succ a_k$ , then  $a_i \succ a_k$
- if  $a_i \sim a_j$  and  $a_j \sim a_k$ , then  $a_i \sim a_k$

with  $a_i, a_j, a_k \in \mathcal{A}$ .

For three choice alternatives the preferences orders and corresponding utilities are given as follow

- $a_1 \succ a_2 \succ a_3 \rightarrow u(a_1) > u(a_2) > u(a_3)$
- $a_1 \succ a_3 \succ a_2 \rightarrow u(a_1) > u(a_3) > u(a_2)$
- $a_2 \succ a_1 \succ a_3 \rightarrow u(a_2) > u(a_1) > u(a_3)$
- $a_2 \succ a_3 \succ a_1 \rightarrow u(a_2) > u(a_3) > u(a_1)$
- $a_3 \succ a_1 \succ a_2 \rightarrow u(a_3) > u(a_1) > u(a_2)$
- $a_3 \succ a_2 \succ a_1 \rightarrow u(a_3) > u(a_2) > u(a_1)$
- $a_1 \succ a_2 \sim a_3 \rightarrow u(a_1) > u(a_2) = u(a_3)$
- $a_1 \sim a_2 \succ a_3 \rightarrow u(a_1) = u(a_2) > u(a_3)$
- $a_2 \succ a_1 \sim a_3 \rightarrow u(a_2) > u(a_1) = u(a_3)$
- $a_2 \sim a_3 \succ a_1 \rightarrow u(a_2) = u(a_3) > u(a_1)$
- $a_3 \succ a_1 \sim a_2 \rightarrow u(a_3) > u(a_1) = u(a_2)$
- $a_3 \sim a_1 \succ a_2 \rightarrow u(a_3) = u(a_1) > u(a_2)$
- $a_1 \sim a_2 \sim a_3 \rightarrow u(a_1) = u(a_2) = u(a_3)$

**Proposition 1.2.3.** For paired comparison data on three choice alternatives  $a_1, a_2, a_3$ , with  $p_{ij} = Q(a_i \succeq a_j)$ , there exists a joint distribution  $\mathcal{P}$  over  $u \in [0, 1]^3$  such that

$$p_{ij} = \mathcal{P}(u_i \geq u_j), (i, j) = (1, 2), (2, 3), (3, 1) \quad (1.2.3)$$

if and only if

$$1 \leq p_{12} + p_{23} + p_{31} \leq 3. \quad (1.2.4)$$

*Proof.* Assume first that there exists  $\mathcal{P}$  such that equation (1.2.3) holds. For  $p_{12}, p_{23}, p_{31}$  it follows that

$$\begin{aligned}
p_{12} &= \mathcal{P}(u_1 > u_2 > u_3) + \mathcal{P}(u_1 > u_3 > u_2) + \mathcal{P}(u_3 > u_1 > u_2) \\
&+ \mathcal{P}(u_1 > u_2 = u_3) + \mathcal{P}(u_3 > u_1 = u_2) + \mathcal{P}(u_3 = u_1 > u_2) \\
&+ \mathcal{P}(u_1 = u_2 = u_3) \\
p_{23} &= \mathcal{P}(u_1 > u_2 > u_3) + \mathcal{P}(u_2 > u_1 > u_3) + \mathcal{P}(u_2 > u_3 > u_1) \\
&+ \mathcal{P}(u_1 = u_2 > u_3) + \mathcal{P}(u_1 > u_2 = u_3) + \mathcal{P}(u_2 = u_3 > u_1) \\
&+ \mathcal{P}(u_1 = u_2 = u_3) \\
p_{31} &= \mathcal{P}(u_3 > u_1 > u_2) + \mathcal{P}(u_2 > u_3 > u_1) + \mathcal{P}(u_3 > u_2 > u_1) \\
&+ \mathcal{P}(u_2 > u_3 = u_1) + \mathcal{P}(u_3 = u_1 > u_2) + \mathcal{P}(u_2 = u_3 > u_1) \\
&+ \mathcal{P}(u_1 = u_2 = u_3). \tag{1.2.5}
\end{aligned}$$

Summing  $p_{12}, p_{23}, p_{31}$  gives

$$\begin{aligned}
p_{12} + p_{23} + p_{31} &= 1 + \mathcal{P}(u_1 > u_2 > u_3) + \mathcal{P}(u_3 > u_1 > u_2) \\
&+ \mathcal{P}(u_2 > u_3 > u_1) + \mathcal{P}(u_1 > u_2 = u_3) + \mathcal{P}(u_3 = u_1 > u_2) \\
&+ \mathcal{P}(u_2 = u_3 > u_1) + 2\mathcal{P}(u_1 = u_2 = u_3) \leq 3. \tag{1.2.6}
\end{aligned}$$

This gives the first part of the proof. The maximal value of three for (1.2.6) is obtained when  $\mathcal{P}(u_1 = u_2 = u_3) = 1$  and the minimal value of one is obtained when the probabilities  $\mathcal{P}(u_1 > u_2 > u_3)$ ,  $\mathcal{P}(u_3 > u_1 > u_2)$ ,  $\mathcal{P}(u_2 > u_3 > u_1)$ ,  $\mathcal{P}(u_1 > u_2 = u_3)$ ,  $\mathcal{P}(u_3 = u_1 > u_2)$ ,  $\mathcal{P}(u_2 = u_3 > u_1)$ ,  $\mathcal{P}(u_1 = u_2 = u_3)$  are all zero. With non-strict preference we do not have  $p_{ij} = 1 - p_{ji}$ . However, the above argument will also apply mutatis mutandis for  $p_{13} + p_{32} + p_{21}$ .

Now assume that equation (1.2.4) holds. We show that there exists a distribution  $\mathcal{P}$  over  $u \in [0, 1]^3$  such that equation (1.2.3) holds. We can write the probabilities  $p_{12}, p_{23}, p_{31}$  as

$$\begin{aligned}
p_{12} &= \mathcal{P}(u_1 > u_2) + \mathcal{P}(u_1 = u_2) \\
p_{23} &= \mathcal{P}(u_2 > u_3) + \mathcal{P}(u_2 = u_3) \\
p_{31} &= \mathcal{P}(u_3 > u_1) + \mathcal{P}(u_3 = u_1). \tag{1.2.7}
\end{aligned}$$

Let  $\alpha \times 100\%$ ,  $0 \leq \alpha \leq 1$  of our stakeholders have strict preferences and the other  $(1 - \alpha) \times 100\%$  of our stakeholders equally prefer all three choice alternatives. Let the sum of the probabilities of the strict preferences from the right hand side of (1.2.7) be  $\beta$  then by an obvious extension of proposition 1.2.1:

$$\alpha \leq \beta \leq 2\alpha. \tag{1.2.8}$$



Similarly summing the probabilities of the equivalence preferences gives

$$\mathcal{P}(u_1 = u_2) + \mathcal{P}(u_2 = u_3) + \mathcal{P}(u_3 = u_1) = 3 - 3\alpha. \quad (1.2.9)$$

Since  $\alpha$  is between zero and one,  $0 \leq \beta \leq 2$ . By assumption, summing the left hand side of (1.2.7) gives

$$p_{12} + p_{23} + p_{31} = \beta + 3 - 3\alpha = \gamma, 1 \leq \gamma \leq 3. \quad (1.2.10)$$

To prove that there exists a distribution over the utility values we only have to show that for all  $\gamma$ ,  $1 \leq \gamma \leq 3$  there exist an  $\alpha$ , with  $0 \leq \alpha \leq 1$  and  $\beta$  with  $0 \leq \beta \leq 2$ . Because we deal with linear inequalities, it suffices to consider  $\gamma = 1$  and  $\gamma = 3$ . For  $\gamma = 1$  it follows that

$$\begin{aligned} 1 &= \beta + 3 - 3\alpha \\ \beta &= 3\alpha - 2 \\ \frac{2}{3} \leq \alpha \leq 1 &\rightarrow 0 \leq \beta \leq 1. \end{aligned} \quad (1.2.11)$$

For  $\gamma = 3$  it follows that

$$\begin{aligned} 3 &= \beta + 3 - 3\alpha \\ \beta &= 3\alpha \\ \alpha = 0 &\rightarrow \beta = 0. \end{aligned} \quad (1.2.12)$$

□

We have to note that proposition 1.2.3 is only valid when the distribution over utility values can be modeled as a discrete distribution. For continuous distributions the probability  $\mathcal{P}(u_i = u_j)$  will always be zero.

Necessary and sufficient conditions for the existences of a random utility function for more than three choice alternatives have not been found, but according to [22] Prof. T. Motzkin proved that proposition 1.2.1 is a sufficient condition for less than six choice alternatives.

### 1.3 Deriving a Random Utility Function using Probabilistic Inversion

A response  $r$  is defined as a function on the stakeholders  $S$ . If the stakeholders are rational and orientable in the sense of Savage, then we could equally well think of  $r$  as a function defined on the utility vectors  $u_S \subset [0, 1]^A$  which are realized by members of  $S$ . Let  $Q_k$  denote the distribution over responses  $r_k$  induced by a

distribution  $P$  over stakeholders  $\mathcal{S}$  and let  $Q = (Q_1, \dots, Q_K)$ . In the case of *strict preference order responses* with  $D_k = \{a_{k_1}, \dots, a_{k_j}\}$ ,  $r_k = \pi \in D_k!$  we would have:

$$\begin{aligned} Q_k(\pi \in D_k!) &= Q_k(\pi^{-1}(1) \succ \dots \succ \pi^{-1}(j)) \\ &= P(s \in \mathcal{S} | \pi^{-1}(1) \succ_s \dots \succ_s \pi^{-1}(j)). \end{aligned} \quad (1.3.1)$$

In analyzing discrete choice data, it is natural to consider the population of stakeholders as a random sample from a virtual population, whose utilities we wish to characterize. In this case  $P$  is simply the counting measure and

$$Q_k(\pi^{-1}(1) \succ \dots \succ \pi^{-1}(j)) = \frac{|(s \in \mathcal{S} | \pi^{-1}(1) \succ_s \dots \succ_s \pi^{-1}(j))|}{|\mathcal{S}|}. \quad (1.3.2)$$

Our problem is to find a distribution  $\mathcal{P}$  over  $u \in [0, 1]^N$  which reproduces  $Q$ ; that is

$$\mathcal{P}(u(\pi^{-1}(1)) \geq \dots \geq u(\pi^{-1}(j))) = Q_k(\pi^{-1}(1) \succ \dots \succ \pi^{-1}(j)); \quad (1.3.3)$$

$$D_k = \{a_{k_1}, \dots, a_{k_j}\}, \pi \in D_k!, k = 1 \dots K. \quad (1.3.4)$$

For *strict preference response*, the formulations are a bit simpler;  $r_k \in D_k$ , and

$$Q_k(r_k) = P(s \in \mathcal{S} | r_k(s) \succ_s a_{k_i}; a_{k_i} \neq r_k(s)); \quad (1.3.5)$$

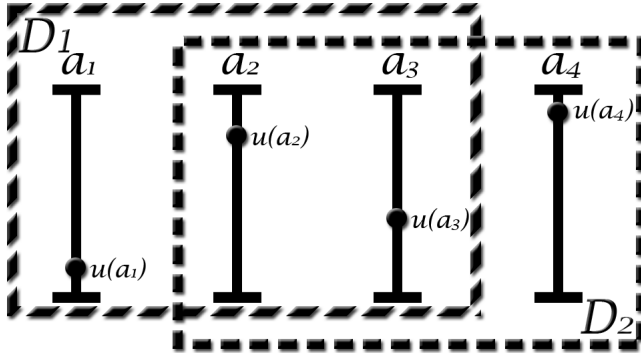
$$\mathcal{P}(u \in [0, 1]^A | u(a_{k_i}) = \max\{u(a_{k_j}) | a_{k_j} \in D_k\}) = Q_k(a_{k_i}). \quad (1.3.6)$$

One recognizes a common form to all these problems, namely, we have a set functions  $r = (r_1, \dots, r_K)$  from the set of possible utility vectors to the set of possible responses, we have distributions over responses generated by the discrete choice data  $Q = (Q_1, \dots, Q_K)$ , and we wish to find a distribution over utility values whose "push forward" distribution through  $r$  coincides with  $Q$ . In other words, we wish to invert  $r$  at  $Q$ . This operation is termed *probabilistic inversion*; a formal definition and intuitive sketch of solution algorithms are given in the following sub section.

### 1.3.1 From Stakeholders' Preference to Random Utility

To obtain an intuitive understanding of the solution algorithms for probabilistic inversion, this section steps through a simple example. Figure (1.3.1) illustrates a mental projection of a stakeholder  $s$  faced with two overlapping groups of choice alternatives,  $D_1$  and  $D_2$ . In this simple example, the stakeholder has to choose one most preferred alternative from each set. With the utilities as shown,  $s$  prefers alternative  $a_2$  from subset  $D_1$  and alternative  $a_4$  from subset  $D_2$ . Another stakeholder might arrange the four alternatives differently on the utility scale, leading to other responses. In practice we can't observe the utility values that stakeholders assign to the alternatives, but we do observe their preferences in terms

**Figure 1.3.1:** Response to  $D_1$  and  $D_2$ :  $u_s = (u_s(a_1), u_s(a_2), u_s(a_3), u_s(a_4))$ ,  $G_1(u_s) = a_2$ ,  $G_2(u_s) = a_4$



of responses to the subsets presented. Suppose that a set of stakeholders induce marginal distributions  $Q$  shown in Table (1.3.1). In other words, in  $D_1$ ,  $a_1$  is preferred by 50% of the stakeholders,  $a_2$  is preferred by 30% of the stakeholders, etc.

**Table 1.3.1:** Marginal distribution  $Q$  over the responses

	$a_1$	$a_2$	$a_3$	$a_4$
$D_1$	0.5	0.3	0.2	N/A
$D_2$	N/A	0.25	0.5	0.25

If we knew the utility function of a stakeholder  $s \in \mathcal{S}$ , then we could obviously predict with certainty how  $s$  would respond to a discrete choice problem. Equivalently, if we are given a vector of utility values over the choice alternatives, we can uniquely determine how a stakeholder with that utility would respond in any discrete choice problem. Our problem is to infer a distribution over (standardized) utility functions given a set of responses from stakeholder population  $\mathcal{S}$ . We solve this problem using a technique called "probabilistic inversion". Probabilistic inversion (PI) is similar to ordinary function inversion: there are sets  $X, Y$ , and a function  $g$  that maps  $X$  into  $Y$ . The quantity  $y \in Y$  is observed and the task then is to find an  $x \in X$  such that  $y = g(x)$ . In the probabilistic setup, the quantities  $x, y$  are random vectors. There are two formulations of probabilistic inversion namely, the measure theoretic version<sup>4</sup> and the random variable version [40] from which we choose the latter.

**Definition 1.3.1.** Let  $\mathbf{X}, \mathbf{Y}$  be random vectors taking values in  $\mathbb{R}^N$  and  $\mathbb{R}^M$  respectively

<sup>4</sup>The measure theoretic approach has been applied before to infer a distribution over the utility values based on a distribution over the preferences[7]

vely. Further let  $G : \mathbb{R}^N \rightarrow \mathbb{R}^M$  be a measurable function.  $\mathbf{X}$  is called a probabilistic inverse of  $G$  at  $\mathbf{Y}$  if  $G(\mathbf{X}) \sim \mathbf{Y}$ , where  $\sim$  means "has the same distribution as". If  $\mathbf{C}$  is a set of random vectors taking values in  $\mathbb{R}^M$ , then  $\mathbf{X}$  is an element of the probabilistic inverse of  $G$  at  $\mathbf{C}$  if  $G(\mathbf{X}) \in \mathbf{C}$ .

There are two main algorithms to carry out PI, namely IPF (Iterative Proportional Fitting) [44],[86],[20] and PARFUM (PARAMeter Fitting for Uncertainty Models) [9],[17],[50]. IPF was first described by Kruithof [44] and later rediscovered by Deming and Stephan [16], and many others. Csiszar [13] proved the convergence of IPF in case of a feasible problem. He shows that if the IPF algorithm converges, then it converges to the unique distribution (called the *I-projection*) which is minimally informative relative of the starting distribution, within the set of feasible distributions. PARFUM was introduced and studied by Cooke [9]. If the problem is feasible, PARFUM converges to a solution which is distinct from the IPF solution. Unlike IPF, PARFUM always converges, and it converges to a solution which minimizes a suitable information functional [17]. The convergence of PARFUM (and its canonical variations) was proved by Matus [58] but has not yet been published. When the problem is feasible IPF is preferred, because of its fast convergence. PARFUM is used when the problem is infeasible, because it insures a solution such that Kullback-Leibler divergence or relative information  $I(G(\mathbf{X})|\mathbf{Y})$  is minimal.

The idea now is to infer from table 1.3.1 a distribution over the utility values given the marginal distributions  $Q$  over the responses using PI. In this example strict preferences are assumed to hold and the probability that  $a_i$  is strictly preferred from  $D_k$  is denoted as  $Q_{k,i}$ .  $\mathcal{P}$  denotes the distribution over utility values. For the diffuse initial distribution we take  $u_1, u_2, u_3, u_4$  to be independent and uniformly distributed on  $[0, 1]$ . This distribution would then yield the following distribution over responses see Table (1.3.2). It does not comply with (1.3.1). Note that we could use other distributions as the initial distribution.

**Table 1.3.2:** Marginal distribution  $Q$  over the responses given uniform distribution

	$a_1$	$a_2$	$a_3$	$a_4$
$D_1$	1/3	1/3	1/3	N/A
$D_2$	N/A	1/3	1/3	1/3

In this case it is possible to find a distribution  $\mathcal{P}$  over the utility values  $u_1, u_2, u_3, u_4$  with either IPF or PARFUM such that this distribution complies with the distribution over the responses  $Q$ . As mentioned, IPF and PARFUM are sample based algorithms for obtaining a probabilistic inverse. These algorithms re-weight samples from a starting distribution to get a distribution over the samples satisfying the constraints (1.3.1). We first draw a number of samples from the starting distributions and then compute the responses to  $D_1, D_2$  for each sampled utility vector. These constitute the values of the functions  $r_1, r_2$ .

$$r_1(s) = \begin{cases} a_1 & \text{if } u_s(a_1) > u_s(a_2), u_s(a_1) > u_s(a_3) \\ a_2 & \text{if } u_s(a_2) > u_s(a_1), u_s(a_2) > u_s(a_3) \\ a_3 & \text{if } u_s(a_3) > u_s(a_1), u_s(a_3) > u_s(a_2) \end{cases} \quad (1.3.7)$$

$$r_2(s) = \begin{cases} a_2 & \text{if } u_s(a_2) > u_s(a_3), u_s(a_2) > u_s(a_4) \\ a_3 & \text{if } u_s(a_3) > u_s(a_2), u_s(a_3) > u_s(a_4) \\ a_4 & \text{if } u_s(a_4) > u_s(a_2), u_s(a_4) > u_s(a_3) \end{cases} \quad (1.3.8)$$

Note that  $r_1, r_2$  constitute the measurable function  $G$  from definition 1.3.1.

For demonstration purposes we use ten samples, but a far greater number of samples is needed in real applications. Table (1.3.3) shows ten samples for  $u_1, u_2, u_3, u_4$  from a uniform distribution together with the computed outputs  $r_1, r_2$ .

**Table 1.3.3:** Ten input and output samples

Sample	$u_1$	$u_2$	$u_3$	$u_4$	$r_1$	$r_2$
1	0.6047	0.13987	0.8202	0.39849	$a_3$	$a_3$
2	0.20205	0.34152	0.47065	0.88651	$a_3$	$a_4$
3	0.11747	0.78388	0.81113	0.36028	$a_3$	$a_3$
4	0.1898	0.25268	0.04756	0.84957	$a_2$	$a_4$
5	0.86156	0.89332	0.20379	0.25159	$a_2$	$a_2$
6	0.14059	0.09522	0.30707	0.28061	$a_3$	$a_3$
7	0.29232	0.20926	0.73012	0.36256	$a_3$	$a_3$
8	0.87431	0.65964	0.42908	0.31673	$a_1$	$a_2$
9	0.36005	0.08888	0.12888	0.03023	$a_1$	$a_3$
10	0.31374	0.82145	0.00599	0.59636	$a_2$	$a_2$

The samples  $(u_1(l), u_2(l), u_3(l), u_4(l), r_1(l), r_2(l))$ , on the  $l$ -th sample ( $l$ -th virtual stakeholder), are drawn from the starting joint distribution  $\mathcal{P}^0$ . Each sample has probability 0.1 under  $\mathcal{P}^0$ . The successive joint distributions obtained after  $m$ -th iterate of IPF or PARFUM will be denoted by  $\mathcal{P}^m$ .

Next we compute the marginal distributions for outputs of  $r_1$  and  $r_2$

$$\mathcal{P}^0(r_1 = a_1), \mathcal{P}^0(r_1 = a_2), \mathcal{P}^0(r_1 = a_3),$$

$$\mathcal{P}^0(r_2 = a_2), \mathcal{P}^0(r_2 = a_3), \mathcal{P}^0(r_2 = a_4)$$

which are presented in table (1.3.4). Evidently these probabilities do not comply with the target probabilities in (1.3.1). Large sample fluctuations with only 10 samples cause large deviations table (1.3.2).

**Table 1.3.4:** Marginal distribution  $Q$  over the responses given  $\mathcal{P}^0$

	$a_1$	$a_2$	$a_3$	$a_4$
$D_1$	0.2	0.3	0.5	N/A
$D_2$	N/A	0.3	0.5	0.2

The  $I$ -projection of a given distribution onto a convex set of distributions is the element of that convex set which is minimally informative with respect to the

given distribution. The IPF procedure successively  $I$ -projects onto each margin, and repeats until convergence is reached. If the problem is feasible IPF converges to a  $\mathcal{P}^*$  which satisfies all constraints and is minimally informative with respect to the starting distribution  $\mathcal{P}^0$  [13]. PARFUM on the other hands averages the  $I$ -projections of each margin to obtain the next iterate. It is not difficult to prove with Lagrange multipliers [13] that the  $I$ -projection of a distribution  $\mathcal{P}^0$  onto the margins of  $r_1$  is given by (1.3.9), where  $Q_{k,i}$  is the  $(k, i)$  entry of Table (1.3.1).

$$I_{r_1}(\mathcal{P}^0) = I_{r_1=a_3}(I_{r_1=a_2}(I_{r_1=a_1}(\mathcal{P}^0))), \quad (1.3.9)$$

with

$$I_{r_k=a_i}(\mathcal{P}_l^0) = \begin{cases} \mathcal{P}_l^0 * \frac{Q_{k,i}}{\mathcal{P}^0(r_k=a_i)} & , r_k(l) = \{a_i\} \\ \mathcal{P}_l^0 & , r_k(l) \neq a_i \end{cases} . \quad (1.3.10)$$

The  $I$ -projection of  $\mathcal{P}^0$  onto the margins of  $r_2$  is computed in the same way as  $r_1$ , but  $\mathcal{P}^0$  replaced by  $I_{r_1}(\mathcal{P}_l^0)$ . Table (1.3.5) shows how an  $I$ -projection of  $\mathcal{P}^0$  onto the margins of  $r_1$  is computed. Note that only the third column are weights that sum to 1, as (1.3.9) requires cycling through all values in the range of  $r_1$ .

**Table 1.3.5:**  $I$ -projection of the margin of  $r_1$ ;  $I_{1,2} \circ I_{1,1}$  denotes  $I_{r_1=a_2} \circ I_{r_1=a_1}(\mathcal{P}^0)$ , etc.

$I_{r_1=a_1}(\mathcal{P}^0)$	$I_{1,2} \circ I_{1,1}$	$I_{1,3} \circ I_{1,2} \circ I_{1,1}$
0.1	0.1	$\frac{0.2}{0.5} * 0.1 = 0.04$
0.1	0.1	$\frac{0.2}{0.5} * 0.1 = 0.04$
0.1	0.1	$\frac{0.2}{0.5} * 0.1 = 0.04$
0.1	$\frac{0.3}{0.3} * 0.1 = 0.1$	0.1
0.1	$\frac{0.3}{0.3} * 0.1 = 0.1$	0.1
0.1	0.1	$\frac{0.2}{0.5} * 0.1 = 0.04$
0.1	0.1	$\frac{0.2}{0.5} * 0.1 = 0.04$
$\frac{0.5}{0.2} * 0.1 = 0.25$	0.25	0.25
$\frac{0.5}{0.2} * 0.1 = 0.25$	0.25	0.25
0.1	$\frac{0.3}{0.3} * 0.1 = 0.1$	0.1

The  $I$ -projections of  $\mathcal{P}^0$  onto  $r_1$ , and the result of  $I$ -projecting that first projection onto  $r_2$  are respectively:

(0.04, 0.04, 0.04, 0.1, 0.1, 0.04, 0.04, 0.25, 0.25, 0.1) and

(0.0488, 0.0714, 0.0488, 0.1786, 0.0556, 0.0488, 0.0488, 0.1389, 0.3049, 0.0556). The next joint distribution  $\mathcal{P}^1$  is equal to last  $I$ -projection.

$$\mathcal{P}^1 = (0.0488, 0.0714, 0.0488, 0.1786, 0.0556, 0.0488, 0.0488, 0.1389, 0.3049, 0.0556). \quad (1.3.11)$$

The marginal distributions for  $r_1, r_2$  given several IPF iteration steps are presented in Table (1.3.6).

**Table 1.3.6:** Marginal distributions  $r_1, r_2$

Step $m$	$r_1 = a_1$	$r_1 = a_2$	$r_1 = a_3$	$r_2 = a_2$	$r_2 = a_3$	$r_2 = a_4$
1	0.4437669	0.2896825	0.2665505	0.25	0.5	0.25
5	0.4998888	0.3001261	0.1999851	0.25	0.5	0.25
10	0.4999959	0.3000048	0.1999993	0.25	0.5	0.25
15	0.4999998	0.3000002	0.2	0.25	0.5	0.25
17	0.5	0.3	0.2	0.25	0.5	0.25

After 17 iterations IPF has converged. Let  $\mathcal{P}^{IPF}$  be the solution of the IPF procedure.  $\mathcal{P}^{IPF}$  is then equal to

$$\mathcal{P}^{IPF} = (0.03625, 0.055, 0.03625, 0.195, 0.0525, 0.03625, 0.03625, 0.145, 0.355, 0.0525). \quad (1.3.12)$$

For PARFUM, the next iterate is computed by first  $I$ -projecting  $\mathcal{P}^0$  separately onto each of the margins  $r_1, r_2$  and then averaging these projections. The next iterate  $\mathcal{P}^1$  is equal to

$$\mathcal{P}^1 = (0.07, 0.0825, 0.07, 0.1125, 0.0917, 0.07, 0.07, 0.1667, 0.175, 0.0917) \quad (1.3.13)$$

The marginal distributions for  $r_1, r_2$  given several PARFUM iteration steps are presented in Table (1.3.7). After 75 iterations PARFUM converges. The PARFUM solution is then equal to

**Table 1.3.7:** Marginal distributions  $r_1, r_2$

Step $m$	$r_1 = a_1$	$r_1 = a_2$	$r_1 = a_3$	$r_2 = a_2$	$r_2 = a_3$	$r_2 = a_4$
1	0.3416667	0.2958333	0.3625	0.35	0.455	0.195
5	0.4744914	0.2919279	0.2335807	0.2847194	0.4803188	0.2349619
25	0.5000717	0.2999113	0.200017	0.2500172	0.4999107	0.2500721
50	0.5000018	0.2999979	0.2000003	0.2500003	0.499998	0.2500017
75	0.5	0.3	0.2	0.25	0.5	0.25

$$\mathcal{P}^{PARFUM} = (0.0363, 0.0547, 0.0363, 0.1953, 0.0524, 0.0363, 0.0363, 0.1453, 0.3547, 0.0524) \quad (1.3.14)$$

As expected IPF converges faster to a solution than PARFUM. Note that the sample weights obtained from IPF (1.3.12) are slightly different those obtained using PARFUM (1.3.14). The utilities of the choice alternatives under IPF and PARFUM are also close (see Tables 1.3.8, 1.3.9). The resulting joint distribution over the choice alternatives induces correlations, as shown in Table (1.3.10) for IPF<sup>5</sup>. Thus a stakeholder who values  $a_2$  highly is also likely to value  $a_1$  highly, but little can be said about his/her valuation of  $a_4$ . More information on iterative methods for probabilistic inversion may be found in [50].

<sup>5</sup>The correlation matrix (1.3.10) is not semi-positive definite due to rounding and the small number

**Table 1.3.8:** Means and Standard Deviations of Utility Values using IPF

	$a_1$	$a_2$	$a_3$	$a_4$
Mean	0.4063	0.3298	0.2509	0.3664
Standard Deviation	0.2505	0.2797	0.2354	0.3235

**Table 1.3.9:** Means and Standard Deviations of Utility Values using PARFUM

	$a_1$	$a_2$	$a_3$	$a_4$
Mean	0.4063	0.3298	0.2510	0.3665
Standard Deviation	0.2506	0.2796	0.2356	0.3234

**Table 1.3.10:** Correlation coefficients of the Utility Values using IPF

	$a_1$	$a_2$	$a_3$	$a_4$
$a_1$	1.00	0.78	0.24	0.23
$a_2$	0.78	1.00	0.69	0.16
$a_3$	0.24	0.69	1.00	0.60
$a_4$	0.23	0.16	0.60	1.00

## 1.4 Multi Criteria Decision Making and Probabilistic Inversion

In many applications of stakeholders' preferences, we want to model the utility values as functions of underlying physical variables. The paradigm case is Multi Attribute Utility Theory (MAUT) where utility is expressed as a weighted combination of physical attributes, such as price, weight, reliability, maintainability, etc. The reservations regarding standard utility modeling expressed in the first section can be dispelled to some extent within the probabilistic inversion approach.

First, we may assume that the utility of stakeholder  $s$  for alternative  $a_i$ ,  $u_s(a_i)$  can be expressed as some function

$$u_s(a_i) = \Phi(c_i, \omega_s), \quad (1.4.1)$$

where  $c_i$  is a vector of 'criteria scores' which depend on  $i$  but not on  $s$ , and  $\omega_s$  is a vector of parameters which depend on  $s$  but not on  $i$ . The population of stakeholders  $\mathcal{S}$  would be described by a distribution over  $\omega_s$ . The most familiar form is the standard MAUT expression:

$$u_s(a_i) = \sum_{j=1}^M \omega_{s,j} \times c_{i,j}. \quad (1.4.2)$$

MAUT assumes that the  $\omega$  are normalized weights. The solution algorithms using IPF and PARFUM proceed exactly as before: we begin with a diffuse starting distribution over  $\omega$  from which a large number of samples are drawn. Using

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of samples used.



(1.4.2) we compute the joint distribution of utility values associated with the starting distribution. IPF and/or PARFUM are applied to re-weight the starting distribution to comply with the discrete choice data. We hasten to add that a wide variety of functional forms would be tractable. For example, we might add quadratic and interaction terms of arbitrary order to (1.4.2) without compromising solvability. Constraints on the parameters  $\omega$ , (non-negativity, normalization) can also be imposed. Sampling the resulting joint distribution of  $\omega$  we obtain the joint distribution of utilities for all alternatives, characteristic for  $\mathcal{S}$ . Note that no assumption regarding the dependence of utility values across  $\mathcal{S}$  is imposed; rather, dependencies emerge from the fitting algorithms themselves. Of course the simple linear form (1.4.2) has distinct advantages; because of the linearity of expectation, the expected utility of an alternative can be simply computed by plugging in the expected values of  $\omega$ .

## 1.5 Model Validation

To exploit the modeling freedom afforded by probabilistic inversion, and to conform with sound science, it is essential to evaluate and validate model forms. The near absence of validation has rendered the field of utility theory more parochial than scientific. We distinguish five levels of model validation for MCDM.

1. Is the model logically consistent with the discrete choice data?
2. Is the discrete choice data consistent with Savage rationality, that is, is there a distribution over utilities that recovers the distribution over the preferences?
3. Does the model recover the preferences from the discrete choice data (in-sample validation)?
4. Can the MCDM utility model fitted on part of the data predict the rest of the data (out-of-sample validation)?
5. Does the MCDM model predict preferences of fresh stakeholders on fresh alternatives (Fresh alternative/stakeholder validation)?

The extent to which these levels are possible depends on the form of the discrete choice data. Many other features also influence the choice of data format. For example, in the nanotechnology enabled food study, we are especially interested in predicting high and low risk scenarios. In the health states application, in contrast, we are interested in valuing all health states without focusing on the very good or very bad.

Three discrete choice formats have been tested with respect to the five levels of validation:

- Paired comparison
- Top/bottom rankings
- Rank overlapping subsets

With paired comparisons, logical consistency (1) is checked with circular triads. Savage rationality (2) can be checked by checking the Marschak [57] necessary condition - or the new condition for non strict preference from proposition 1.2.3. The MCDM utility model can be validated in-sample(3) as well as out of sample (4) and (5) fresh alternative/stakeholder validation. In previous studies[70, 73] the paired comparison format was found to pose a very heavy assessment burden. This format has therefore not been used in the studies for this thesis.

Top/bottom ranking (Ecosystems prioritization [71, 90] and in the nanotechnology enabled food safety [24] studies): Level (1) can be checked by checking violations of dominance, if there are dominated scenarios. (2) is difficult to check, as utilities of unranked scenarios are indeterminate. Levels (3), (4) are performed for both studies. Level (5) was performed in the nanotechnology application during an experts's workshop enlisting fresh experts. Evidently, fresh alternative/stakeholder validation is very resource intensive. These studies are described in the chapters 4 and 6.

Rank overlapping subsets (Health State valuation study [72]): Level (1) validation is done by checking preference reversal, and levels (2), (3), and (4) are done as well, see chapter 5.

# Independence of Irrelevant Alternatives

## 2.1 Introduction

With discrete choice analysis it is possible to predict shares of a given set of choice alternatives based on preferences of a group of respondents or stakeholders. Examples of such exercises are predicting the share of transportation modes or shares of a new product [61, 59, 33, 77, 96].

Several models can be used to translate group preferences into shares. Among these models are the Logit or Bradley-Terry model[5, 93, 25]. The Logit model offers a closed form solution which makes predicting the shares relatively easy. Besides the computational benefits of the Logit model, it also has some drawbacks when used in real life applications. The pros and cons of these models have been debated in terms of the Independence of Irrelevant Alternatives (IIA) assumption. As elaborated in the following section, IIA implies that the ratio of probabilities of choosing any two alternatives is independent of other alternatives. This implies that adding a new alternative does not alter the "odds ratio" of choosing between two alternatives already present.

Consider the *blue-bus, red-bus* example[15]. Commuters initially face a decision between two modes of transportation namely, the car and the bus. Let the probability of commuters choosing the car equal 0.5 and the probability of choosing the bus equal 0.5. Thus the odds ratio of the car and the bus is 1. Now suppose that the bus company paints half of the buses red and the other half blue. Assuming bus commuters do not care about the color of the bus, consumers are expected to choose between bus and car still with equal probability, so the probability of car should remain 0.5, while the probabilities of choosing a bus (red or blue) is 0.5. IIA implies that this is not the case: for the odds ratio between car

and red bus to be preserved, the new probabilities for choosing the car, the red bus, or the blue bus must all be 0.33. Intuitively, the problem with the IIA axiom is that it fails to account for the fact that commuters see the red- and blue bus as the same type of transportation.

In this chapter we will direct our focus to the IIA assumption and its implications. We show that the red-blue bus conundrum is not so much about IIA, but results from confusing strict and non-strict preference. To resolve the conundrum, it is essential to distinguish *probabilistic indifference from individual preference indifference*. If 50% of the stakeholder population strictly prefer alternative A to alternative B, then the chance of a random stakeholder choosing A when offered a choice of  $\{A, B\}$  is 1/2. This is probabilistic indifference. If all stakeholders are indifferent between A and B, and if they choose randomly when offered the choice  $\{A, B\}$ , then the probability of a random stakeholder choosing A is also 1/2. However these two cases are very different. Indeed, if preferences may be non-strict, then the condition in proposition 1.2.1 is not necessary for consistency. A more general result is proved in section 1.2.2. If all preferences are indeed strict then IIA does not lead to paradoxes like the red-blue bus conundrum. IIA may be false, but it is not paradoxical. The discrete choice formalism and solution techniques introduced in chapter one are used to analyse these issues. Indeed, we show that if we admit probabilistic indifference, the red-blue bus example *does* satisfy IIA.

## 2.2 IIA

Following the notation of chapter 1, we denote the set of choice alternatives by  $\mathcal{A} = \{a_1, \dots, a_n\}$ ,  $\mathcal{S}$  the set of stakeholders, and  $\mathcal{D}$  as the set of discrete choice problems generated by  $\mathcal{A}$ . Further let  $D_{\{i,j\}} = \{a_i, a_j\} \in \mathcal{D}$  then  $r_{D_{\{i,j\}}}$  denotes the response function of  $s \in \mathcal{S}$  to  $D_{\{i,j\}}$ . The probability distribution  $Q$  over  $r_{D_{\{i,j\}}}$  is induced by a distribution  $P$  over  $\mathcal{S}$ .

Several formulations of (IIA) are found in the literature. Most of these formulations describe IIA as a condition on the response functions. Basically the IIA condition implies that if a stakeholder for a given set  $D_{\{1,2\}} = \{a_1, a_2\}$  prefers  $a_1$  over  $a_2$  then he also would prefer  $a_1$  over  $a_2$  if faced with an extended set  $D_{\{1,2,3\}} = \{a_1, a_2, a_3\}$ . Luce gave a stochastic formulation of IIA which has led to derivation of the Logit and the Bradley-Terry Luce model [54].

**Definition 2.2.1.** *If  $D$  is a discrete choice problem on  $\mathcal{A}$  with strict response, let  $D_{ij} = \{a_i, a_j\}$  and let  $D_{ij+} \in \mathcal{D}$  be a superset of  $D_{ij}$ , then IIA holds if*

$$\frac{Q(r_{ij} = a_i)}{Q(r_{ij} = a_j)} = \frac{Q(r_{ij+} = a_i)}{Q(r_{ij+} = a_j)}$$

Definition 2.2.1 on strict responses leads to the following condition on the distribution of the utility values  $\mathcal{P}$ .

$$\frac{\mathcal{P}(u(a_i) > u(a_j))}{\mathcal{P}(u(a_j) > u(a_i))} = \frac{\mathcal{P}(\forall_{a_k \in D_{ij+}} u(a_i) > u(a_k))}{\mathcal{P}(\forall_{a_k \in D_{ij+}} u(a_j) > u(a_k))} \quad (2.2.1)$$

with  $\mathcal{P}(u(a_i) > u(a_j)), \mathcal{P}(\forall_{a_k \neq a_i \in D_{ij+}} u(a_i) > u(a_k)) \neq 0 \forall a_i, a_j, a_k \in \mathcal{A}$ .

Marschak [57] showed that for a distribution  $\mathcal{P}$  satisfying equation (2.2.1), there exist a function  $v : \mathcal{A} \mapsto \mathbb{R}_+$ , random variables  $V(a_i), a_i \in \mathcal{A}$  and a function  $\phi : \mathbb{R} \mapsto [0, 1], \phi(-\infty) = 0, \phi(0) = 1/2, \phi(\infty) = 1$  such that (recall, under  $\mathcal{P}, u(a_i)$  is a random variable):

1.  $u(a_i) = v(a_i) + V(a_i), E(V(a_i)) = 0,$  and  $v(a_i) > 0$
2.  $\mathcal{P}(u(a_i) \geq u(a_j)) = \phi(v(a_i) - v(a_j)),$
3.  $\mathcal{P}(V(a_i) - V(a_j) \leq \lambda) = \phi(\lambda)$
4.  $\mathcal{P}(\forall_{a_k \in D_{ij+}} u(a_j) \geq u(a_k)) = \frac{v(a_i)}{\sum_{a_k \in D_{ij+}} v(a_k)}$
5.  $Q_{12} * Q_{23} * \dots * Q_{n-1,n} * Q_{n1} = Q_{21} * Q_{32} * \dots * Q_{n,n-1} * Q_{1n}$  with  $Q_{ij} = Q(r_{ij} = \{a_i\}), 0 < Q_{ij} < 1$

The first three conditions ensure a probability distribution over the utility values and the last one ensures that (2.2.1) hold. By putting  $v(a_i) = e^{w(a_i)}$  the form of the distribution becomes:

$$\phi(\lambda) = \frac{1}{1 + e^{-\lambda}}. \quad (2.2.2)$$

Satisfying the condition in proposition 1.2.1 however is not a sufficient condition for the existence of a probability distribution satisfying (2.2.1). For example take let  $\mathcal{A} = \{a_1, a_2, a_3\}$  with simple paired comparison, and  $Q_{12} = Q_{23} = 0.75, Q_{31} = 0.25$ ; then it satisfies proposition 1.2.1, but it fails (2.2.1).

The distribution that follows from (2.2.1) has its advantages and disadvantages. One of the advantages is that this distribution has closed form. The closed form makes it then relatively easy to estimate parameters of the utility function  $v(a_i)$  or the share of  $a_i$  which is equal to the probability that  $a_i$  is preferred to all alternatives in  $\mathcal{A}$ .

As a disadvantage this distribution puts restrictions on the probability values over the responses in addition to proposition 1.2.1. This disadvantage has not been highlighted by many in the literature [57]. Another well known disadvantage of this distribution is the so called *blue-bus, red-bus problem* [15], [8]. In the *blue-bus, red-bus problem* the distribution predicts counter intuitively that a bus company could increase its market share by painting its buses different colors. To cope with this problem McFadden and others [64], [77], [96] introduced the so called *Mixed-Logit model* to capture these dependencies among the utility values

of the alternatives. The dependence structure does not emerge from the data, but is imposed a priori.

According to the discrete choice approach set forth in chapter one, inferring dependence structures from the discrete choice data with probabilistic inversion is preferable to imposing such structures a priori. Because probabilistic inversion yields the entire joint distribution over the utility values, we can compute all moments and dependency structures. In examples like the red-blue bus paradox, the probabilistic inversion must explicitly take account of equivalence in preference. A group of stakeholders is said to be probabilistic indifferent with respect to alternatives  $a_i, a_j$  if 50% strictly prefers  $a_i$  to  $a_j$  and the other 50% strictly prefers  $a_j$  to  $a_i$ . A group of stakeholders is individually indifferent to alternatives  $a_i, a_j$  if these are equivalent in preference for each stakeholder. It may be difficult to distinguish probabilistic indifference and individual preference indifference in discrete choice data whose collection protocols were not specifically designed for this purpose <sup>1</sup>. This, however, is a question of experimental design, and should not lead us to confuse probabilistic and individual preference indifference. Of course, mixtures of probabilistic and individual preference may also arise, which further complicates the issues. The next section demonstrates how probabilistic indifference and individual preference indifference lead to very different conclusions when probabilistic inversion is applied to discrete choice data.

## 2.3 Implications of IIA

Four scenarios that the bus company might face are analyzed below and questions of the bus company (see introduction) are answered for each scenario. We shall see that the answers differ according to whether preferences are strict or non-strict. The choice alternative set  $\mathcal{A}$  will contain three choice alternatives  $\{a_1 = Bus1, a_2 = Bus2, a_3 = Car\}$ . The two bus lines can also be marked as the blue-bus and red-bus as in the example of Debreu[15]. Stakeholders are faced with paired comparisons

$$\mathcal{D} = \{D_{\{1,2\}} = \{a_1, a_2\}, D_{\{2,3\}} = \{a_2, a_3\}, D_{\{3,1\}} = \{a_3, a_1\}\}$$

For a stakeholder faced with  $D_{\{i,j\}}$  he or she might either respond with either  $a_i, a_j$  or  $\{a_i, a_j\}$ .

### 2.3.1 From Preferences to Shares

Before working out the four scenarios we explain how to derive the shares of the three transportation modes using Probabilistic Inversion. We assume that the

<sup>1</sup>As described in Savage [82], strict preference between two alternatives may be detected by supplementing the unchosen alternative with vanishingly small utility increments. Alternatively, intransitivities in pair wise comparison data may indicate indifference.

utility functions of all commuters take value within the unit cube

$(u(a_1), u(a_2), u(a_3)) \in [0, 1]^3$ . If a commuter  $s \in \mathcal{S}$  responds to  $\{a_i, a_j\}$  with  $\{a_i\}$  then it is assumed that  $u(a_i) > u(a_j)$ , and if responded with  $\{a_j\}$  then  $u(a_j) > u(a_i)$ . If a commuter responds with  $\{a_i, a_j\}$  then it is assumed that  $u(a_i) = u(a_j)$ . In formula this gives

$$r_{\{i,j\}}(s) = \begin{cases} a_i & \text{if } u_s(a_i) > u_s(a_j) \\ a_j & \text{if } u_s(a_i) < u_s(a_j) \\ \{a_i, a_j\} & \text{if } u_s(a_i) = u_s(a_j). \end{cases} \quad (2.3.1)$$

The distribution over responses is obtained from the distribution over commuters giving

$$\begin{aligned} Q(r_{\{i,j\}} = a_i) &= \frac{\sum_{s \in \mathcal{S}} 1_{r_{\{i,j\}}(s) = a_i}}{|\mathcal{S}|} \\ Q(r_{\{i,j\}} = a_j) &= \frac{\sum_{s \in \mathcal{S}} 1_{r_{\{i,j\}}(s) = a_j}}{|\mathcal{S}|} \\ Q(r_{\{i,j\}} = \{a_i, a_j\}) &= \frac{\sum_{s \in \mathcal{S}} 1_{r_{\{i,j\}}(s) = \{a_i, a_j\}}}{|\mathcal{S}|}. \end{aligned} \quad (2.3.2)$$

We want to find a distribution  $\mathcal{P}$  over the commuters utility values  $(u(a_1), u(a_2), u(a_3)) \in [0, 1]^3$  such that when plugged into 2.3.1 we observe 2.3.2. As mentioned before this is done using sample re-weighting techniques of Probabilistic Inversion. We start with an initial non-informative distribution over the utility values which is the joint uniform distribution and sample a large number of utility values from it. When sampling from a continuous distribution one would never observe the event  $u_s(a_i) = u_s(a_j)$ . There are a number of ways to deal with this problem. In the first approach one could sample from the continuous uniform distribution and assume that if a stakeholder responds with  $\{a_i, a_j\}$  that there is no noticeable difference in the utility values of  $u_s(a_i), u_s(a_j)$  if there exists a  $\epsilon > 0$  such that

$$a_i \sim_s a_j \rightarrow |u_s(a_i) - u_s(a_j)| < \epsilon, i \neq j$$

In the second approach that we have used one does not need to include an additional dependency of  $\epsilon$  and can simply sample from the discrete uniform distribution and normalize the utility values such that they are between zero and one.

After properly sampling these utility values we obtain a  $\mathcal{P}^*$  using either IPF or PARFUM if the problem is feasible and a solution  $\mathcal{P}^\sim$ , which is as good as possible, with PARFUM if the problem is infeasible. After obtaining this joint distribution over the utility values  $(u(a_1), u(a_2), u(a_3)) \in [0, 1]^3$  we can calculate not only the means, standard deviation, and correlations, but also the probability that  $a_i$  is ranked first or the share of  $a_i$ , which is given as follows

$$p_{a_i \#1} = \mathcal{P}(\forall_{a_k \in \mathcal{A}} u(a_i) \geq u(a_k)), \quad (2.3.3)$$

with  $p_{a_i \#1}$  the share of  $a_i$ .

### 2.3.2 Scenario One

In the first scenario all passengers have strict preference. 60% prefer the car over bus line 1 ( $Q(r_{\{3,1\}} = a_3) = \alpha_{31} = 0.6$ ), 80% prefer the car over bus line 2 ( $Q(r_{\{3,2\}} = a_3) = \alpha_{32} = 0.8$ ), and 45% prefer bus line 2 over bus line 1 ( $Q(r_{\{2,1\}} = a_2) = \alpha_{21} = 0.45$ ). According to proposition 1.2.1 this is a feasible problem so we were able to find a random utility function using IPF, but we would not be able to find a solution satisfying IIA, because one of the constraints is not met ( $\alpha_{12} * \alpha_{23} * \alpha_{31} = 0.55 * 0.2 * 0.6 \neq \alpha_{21} * \alpha_{32} * \alpha_{13} = 0.45 * 0.8 * 0.4$ ). Fig. 2.3.1 illustrates the margins for the utility values for each choice alternative. From the margins we can read how probable certain utility values are for a given choice alternative. From figure 2.3.1 it follows that high utility values for the car are more probable than low values.

The means, standard deviations, and correlations from the transportation modes are given in table 2.3.1.

**Table 2.3.1:** Probabilistic Inversion using IPF First Scenario

$\mu_{B1}$	$\mu_{B2}$	$\mu_{Car}$	$\sigma_{Bus1}$	$\sigma_{B2}$	$\sigma_{Car}$	$\rho_{B1B2}$	$\rho_{B1Car}$	$\rho_{B2Car}$
0.463	0.439	0.600	0.2926	0.2732	0.2724	-0.019	-0.045	0.166

With the joint density  $\mathcal{P}^*$  obtained from IPF we can compute the probability that the car is preferred over both bus lines. This probability is equal to the share of the car:  $p_{Car} = 0.5339$ . Therefore 53.39% of the time the stakeholders will prefer the car over either bus and 46.61% of the time the stakeholders will prefer one of the buses over the car. The share for bus line 1 would be 32.26% and the share of bus line 2 would be 14.35%. If the bus company would cancel bus line 1 then it would lose 26.61% of its share and if it would cancel bus line 2 its share would loss 6.61% of its currently held share<sup>2</sup>.

### 2.3.3 Scenario Two

In scenario two the commuters also have strict preferences and we have probabilistic indifference among all three choice alternatives. Thus 50% strictly prefer the car over bus line 1 ( $Q(r_{\{3,1\}} = a_3) = \alpha_{31} = 0.5$ ), 50% strictly prefer the car over bus line 2 ( $Q(r_{\{3,2\}} = a_3) = \alpha_{32} = 0.5$ ), and 50% strictly prefer bus line 2 over

<sup>2</sup>The drop in share is calculated by subtracting the probability of bus line  $i$  being preferred to the car from the total share of bus lines combined



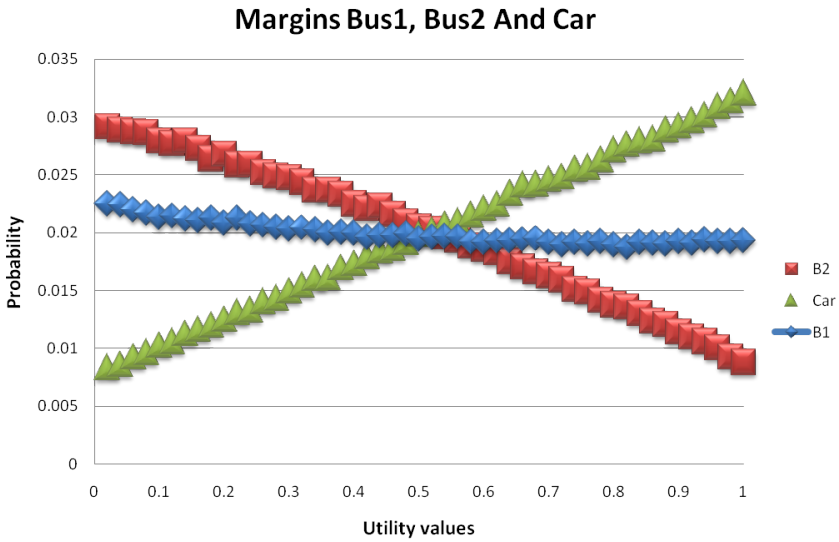


Figure 2.3.1

bus line 1 ( $Q(r_{\{2,1\}} = a_2) = \alpha_{21} = 0.5$ ). In this scenario we could find a solution using both probabilistic inversion and a solution satisfying the IIA constraints. Fig. 2.3.2 shows the margins for the utility values.

The means, standard deviations, and correlations from the transportation modes are given by table 2.3.2 .

Table 2.3.2: Probabilistic Inversion using IPF Second Scenario

$\mu_{B1}$	$\mu_{B2}$	$\mu_{Car}$	$\sigma_{B1}$	$\sigma_{B2}$	$\sigma_{Car}$	$\rho_{B1B2}$	$\rho_{B1Car}$	$\rho_{B2Car}$
0.4999	0.4994	0.4993	0.2887	0.2888	0.2885	0.0004	-0.001	-0.003

The probability  $p_{Car} = 0.33$ , so 33% of the time the stakeholders prefer the car over the bus and 66% of the time the stakeholders prefer the combined bus lines over the car. Canceling either bus line would decrease the share with 16%. Introducing an extra bus line might indeed lead to extra share if the case of the

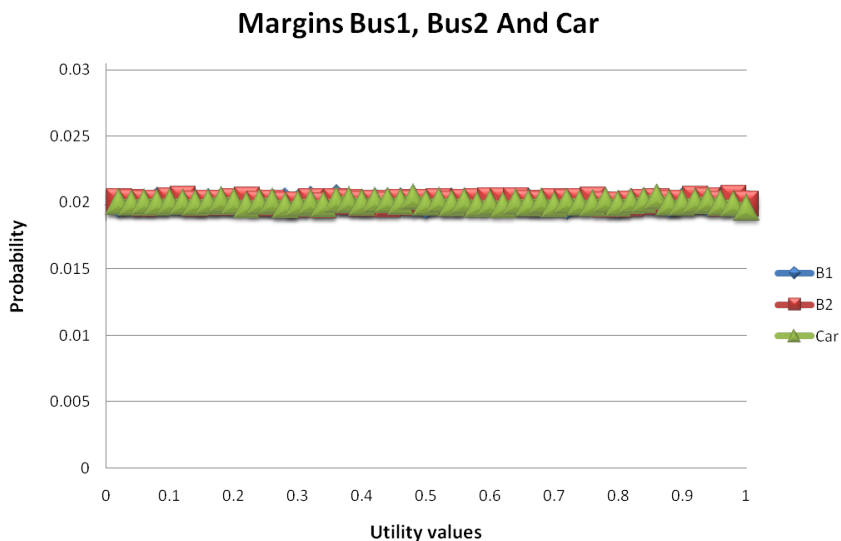


Figure 2.3.2

extra bus line if probabilistic indifference again holds. An extra line would mean an extra mode of transportation in the perception of the stakeholders. Evidently if the number of bus would approach infinity then the share of the bus would approach 100%.

### 2.3.4 Scenario Three

In the third scenario the commuters have strict preferences between the buses and the car and non-strict preferences among the buses. 50% strictly prefer the car over bus line 1 ( $Q(r_{\{3,1\}} = a_3) = \alpha_{31} = 0.5$ ), 50% strictly prefer the car over bus line 2 ( $Q(r_{\{3,2\}} = a_3) = \alpha_{32} = 0.5$ ), and 100% are indifferent about either two bus lines ( $Q(r_{\{2,1\}} = \{a_2, a_1\}) = 1$ ). So  $Q(r_{\{2,1\}} = a_2) = \alpha_{21} = 0$  and  $Q(r_{\{1,2\}} = a_1) = \alpha_{12} = 0$ . Note that the probabilities of scenario 3 satisfy both proposition 1.2.1 and proposition 1.2.3. For strict preferences it follows from proposition 1.2.1 that  $1 \leq \alpha_{12} + \alpha_{23} + \alpha_{31} = 0 + 0.5 + 0.5 = 1$ , where

$\alpha_{ij} = Q(r_{\{i,j\}} = a_i)$  denotes strict preferences. In case of non-strict preferences it follows from proposition 1.2.3 that  $1 \leq p_{12} + p_{23} + p_{31} = 1 + 0.5 + 0.5 = 2 \leq 3$ , where  $p_{ij} = Q(a_i \sim a_j) = Q(r_{\{i,j\}} = a_i) + Q(r_{\{i,j\}} = \{a_i, a_j\})$ . Note that IIA does hold in this case. The probability of choosing the red over the blue bus is 1/2 (everyone is indifferent but if they must choose, they choose randomly). Adding a car doesn't change that. Similarly, the probability that the car is preferred (in this case strictly) over the red bus is 1/2 and doesn't depend on whether the the blue bus is or is not available. This shows that the red-blue bus conundrum results from a failure to distinguish strict and non-strict preference and is not a problem for IIA when strict and non-strict preference are properly distinguished.

Fig. 2.3.3 illustrates the margins for the utility values from the transportation modes.

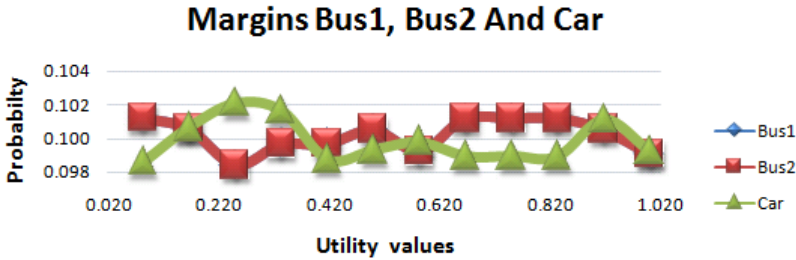


Figure 2.3.3

The means, standard deviations, and correlations from the transportation modes are given by table 2.3.3.

Table 2.3.3: Probabilistic Inversion using IPF Third Scenario

$\mu_{B1}$	$\mu_{B2}$	$\mu_{Car}$	$\sigma_{B1}$	$\sigma_{B2}$	$\sigma_{Car}$	$\rho_{B1B2}$	$\rho_{B1Car}$	$\rho_{B2Car}$
0.4998	0.4998	0.4998	0.289	0.289	0.288	1	0.002	0.002

The probability  $p_{Car} = 0.49748$  - the deviation from 1/2 is of numerical origin. Thus 50% of the time the stakeholders prefer the car over either of the buses. The margins of bus lines in the second and third scenario coincide, but from the correlation coefficient  $\rho_{b1b2}$  of bus line 1 and bus line 2 from third scenario it follows that bus line 1 is not different from bus line 2. Canceling either one of the bus lines wouldn't significantly affect the share of the bus.

### 2.3.5 Scenario Four

In the fourth and final scenario 60% strictly prefer the car over bus line 1 ( $Q(r_{\{3,1\}} = a_3) = \alpha_{31} = 0.6$ ), 80% strictly prefer the car over bus line 2

( $Q(r_{\{3,2\}} = a_3) = \alpha_{32} = 0.8$ ), 100% of the stakeholders were indifferent over either bus lines ( $Q(r_{\{2,1\}} = \{a_2, a_1\}) = 1$ ).

From proposition 1.2.1 it follows that no random utility function exists satisfying these strict preferences:  $\alpha_{12} + \alpha_{23} + \alpha_{31} = 0 + 0.20 + 0.60 = 0.80 < 1$ . However, if forced to choose between bus 1 and bus 2 stakeholders will choose randomly; if we mistake that for strict preference, then  $\alpha_{12} = 0.5$  and a strict preference solution can be found. Mistaking individual indifference for probabilistic indifference will yield paradoxes. According to proposition 1.2.3 there exists a distribution over the utility values, satisfying these non-strict preferences since  $1 \leq p_{12} + p_{23} + p_{31} = 1 + 0.2 + 0.6 = 1.8 \leq 3$ .

The means, standard deviations, and correlations from the transportation modes are given by table 2.3.4.

**Table 2.3.4:** *Probabilistic Inversion using IPF Fourth Scenario*

$\mu_{B1}$	$\mu_{B2}$	$\mu_{Car}$	$\sigma_{B1}$	$\sigma_{B2}$	$\sigma_{Car}$	$\rho_{B1B2}$	$\rho_{B1Car}$	$\rho_{B2Car}$
0.404	0.404	0.608	0.2722	0.2719	0.2717	1	0.1148	0.1164

The margins of the utility values from the transportation modes are given by fig. 2.3.4.

The probability  $p_{Car} = 0.799$ , so 79.9% of the time the stakeholders prefer the car over the bus and 20.1% of the time the stakeholders prefer the combined bus lines over the car.

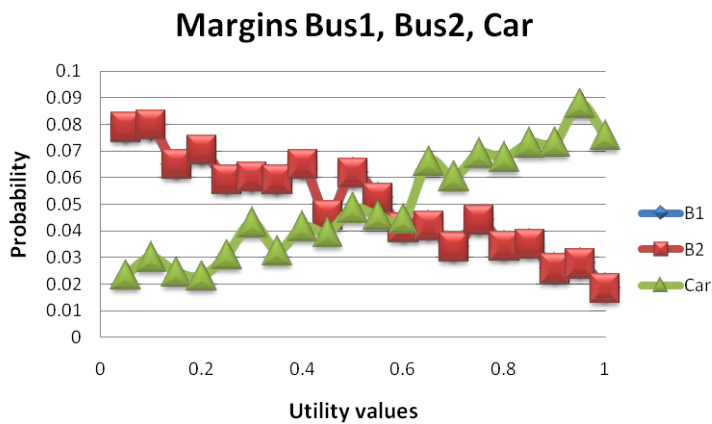


Figure 2.3.4

## 2.4 Conclusion

Scenario two and three of the bus company from the previous showed that group indifference can have two sources. One source can be traced to the fact that half the group can have choice alternative  $a_i$  as response to  $\{a_i, a_j\}$ , and the other half can have choice alternative  $a_j$  as response. In a situation like this, models that are based on the IIA assumption will work fine. Taken into account the red-bus, blue-bus example and scenario two of the example it would simply mean that introducing a new bus or bus line increases the probability of bus being chosen as a transportation mode, which leads to an increase of share.

The other source of indifference is found on an individual level. In other words there are stakeholders in the group that are indifferent about combined buses or bus lines see scenario three and four. In practice there is no way of to know upfront if stakeholders' response will be strict or non-strict so it seems a

good practice to let them express their preferences properly. If in the case of the bus scenarios this was not taken into account there was no way of telling that the two buses are the same in terms of utility values, which would lead to a paradox.

The above emphasizes the fact that on binomial or multinomial choice data (paired comparisons, multiple choices) alone we cannot distinguish strict preference from equivalence in preference. If stakeholders in Scenario three of our examples weren't able to express their indifference properly it might have occurred that  $Q(a_1 \succeq a_2) = Q(a_2 \succeq a_1) = 1$ . According to proposition 1.2.1 this would still yield a distribution over the utility values, but conventional methods would not be able to derive a distribution over utility values.

However when presented with a discrete choice data set that hasn't taken into account non-strict preferences one can test if stakeholders responded at random. As mentioned before the source of inconsistency can be due to expert choosing at random. If choosing at random is due to non-strict preferences then one can use our method to be used to properly analyze the discrete choice data set.

With our formalism and techniques for discrete choice we were able to cope with both sources of indifference without creating a paradox. This formalism and technique for discrete choice is capable of highlighting the dependency structures over the utility values that follow from the responses without the need of defining them beforehand.

# Minimum Information and Independence in Discrete Choice

## 3.1 Introduction

Discrete choice denotes the choice behavior of a group of stakeholders given a set of choice alternatives. The basic assumption made in discrete choice is that the utility over the choice alternatives can be inferred from stakeholders' preferences. Examples of discrete choice exercises are the modeling of purchase behavior of a new car or the selection of a given mode of transportation. The goal of discrete choice is to quantify the (utility) values of the set of choice alternatives based on preferences or selections of stakeholders. To reach this goal two tasks must be carried out. The first task is to model attributes or characteristics of choice alternatives that contribute to utility. For example the purchase of a car depends on the car's price, size, fuel consumption, etc. It is possible to model utility given the choice attributes for a given stakeholder. However it is fool's errand to derive a single utility function for the group of stakeholders or to derive stakeholder specific utility functions[3, 4, 84, 89]. That is where the second task comes in to play. Here the previously derived model is extended with random characteristics to incorporate the fluctuation in stakeholders' utility. The distribution of the random terms is estimated using for example selections, purchases, or orderings given the set of choice alternatives as data. The problem of discrete choice can be formulated as an inverse problem.

There are several types of methods that can deal with stochastic inverse problems. Examples of such methods are Regression[29, 74, 23, 26], Maximum Likelihood[12, 30], Bayesian Updating[38], and Minimal Relative Information[45, 20, 86]. Examples of discrete choice models that use regression or maximum likelihood are the Logit and Probit models[91, 55, 60, 62]. The Logit and Probit

models assume that utility is a composition of choice attributions with some randomly distributed error term. In the Logit model the error terms are generalized extreme value (GEV) distributed and in the Probit the error terms are normally distributed. The advantage of the Logit model is that it has a closed form representation which eases the burden of estimating the coefficients of the choice attributes. On the other hand it suffers from the so called independence of irrelevant alternatives (IIA)[15]. The Probit model does not suffer from IIA, but does not have a closed form. Both models require certain dependency structures of the error terms in order to obtain a solution. So far we've not encountered models that make use of Minimal Relative Information. A literature review did not turn up explicit use of the minimal information principle to discrete choice models, though maximum likelihood methods are closely related to information minimization.[1].

In this chapter we will investigate the derivation of a distribution over utility using minimal relative information subject to marginal constraints in the form of discrete choice data. The type of discrete choice data that will be used is paired comparisons. The problem of finding a minimal relative information distribution is formulated as a constrained optimization problem, which can be solved using either the method of Lagrange or Probabilistic Inversion (PI). In section 3.2 we will use a uniform distribution as the starting distribution and examine the independence assumption. It emerges that PI can find solutions where standard optimization methods will fail due to intractability. In section 3.4 we will use a normal distribution as a starting distribution and compare the solution with the one obtained from Thurstone[91, 92]. We will demonstrate in sections 3.3.3 and 3.3.4 that the dependency structures often assumed for the distribution over the utility values adds additional relative information.

## 3.2 Minimal Relative Information Solution of a Uniform Distribution Without Independence

Let  $\mathcal{A} = \{a_1, \dots, a_N\}$  be the set of choice alternative, with  $N$  choice alternatives, and  $\mathcal{S}$  the group of stakeholders. The preferences of each stakeholder are denoted as  $a_i \succeq_s a_j, s \in \mathcal{S}$ , which implies that  $a_i$  is at least as preferable as  $a_j$  for  $s$ . The probability that  $a_i \succeq a_j$  is equal to the number of stakeholders who preferred  $a_i$  to  $a_j$  divided by the number stakeholders:

$$P(a_i \succeq a_j) = P(s \in \mathcal{S} | a_i \succeq_s a_j) = \frac{\sum_{s=1}^{|\mathcal{S}|} 1_{\{a_i \succeq_s a_j\}}}{|\mathcal{S}|} \quad (3.2.1)$$

Each  $s \in \mathcal{S}$  may be assigned a utility function over choice alternatives that is unique up to a positive affine transformation, i.e. unique up to choice of zero and



unit. As in chapter 1 we assume that our set of stakeholders have utility functions which can be assigned the same unit, and that the utilities over  $\mathcal{A}$  may be represented as standardized  $N$ -vectors taking values in  $[0, 1]$ , that is, as elements of  $[0, 1]^N$ . If nothing is known about what drives the utility values of the choice alternatives we assume a discrete uniform distribution over  $\{\frac{1}{M}, \dots, 1\}^N$ , denoted  $g$ . We seek a joint probability mass function  $f$  for the utilities over  $\mathcal{A}$  that is as close as possible to  $g$  in terms of relative information and that satisfies the following constraints.

$$\begin{aligned} \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} f(u) &= 1 \\ \mathcal{P}(u_i > u_j) &= \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} f(u) 1_{\{u_i > u_j\}} \\ &= Q(s \in \mathcal{S} | a_i \succ_s a_j) \\ &= \alpha_{ij} \\ \alpha_{ij} &\in (0, 1), \forall i \neq j \end{aligned} \tag{3.2.2}$$

$\mathcal{P}$  denotes the probability measure on the utility values and  $Q$  the probability measure over stakeholders' preferences and  $u_i \in \{\frac{1}{M}, \dots, 1\}$  the utility value of choice alternative  $a_i$ .

### 3.2.1 Two Choice Alternatives

For two choice alternatives  $a_1, a_2 \in \mathcal{A}$  and strict responses, the problem of finding a minimum informative probability mass function  $f(u_1, u_2)$  over the utility values, such that  $\sum_{u \in \{\frac{1}{M}, \dots, 1\}^2: u_1 > u_2} f(u) = \alpha$ , can be formulated as follows:

$$\operatorname{argmin}_f I(f|g) = \operatorname{argmin}_f \sum_{u \in \{\frac{1}{M}, \dots, 1\}^2} f(u) \ln \frac{f(u)}{g(u)} \tag{3.2.3}$$

Subject to:

$$\begin{aligned} \sum_{u \in \{\frac{1}{M}, \dots, 1\}^2} f(u) &= 1 \\ \sum_{u \in \{\frac{1}{M}, \dots, 1\}^2: u_1 > u_2} f(u) &= \alpha; 0 < \alpha < 1 \end{aligned} \tag{3.2.4}$$

**Proposition 3.2.1.** *The minimally informative distribution that satisfies 3.2.3 and 3.2.4 is equal to*

$$f^*(u_1, u_2) = \begin{cases} \frac{2\alpha}{M(M-1)}, & u_1 > u_2 \\ \frac{2(1-\alpha)}{M(M+1)}, & u_1 \leq u_2 \\ (u_1, u_2) & \in \{\frac{1}{M}, \dots, 1\}^2 \end{cases} \tag{3.2.5}$$

The proof of (proposition 3.2.1) uses the method of Lagrange multipliers and may be found in the appendix. The relative information of the minimally informative distribution of proposition 3.2.1 is

$$\begin{aligned}
 I(f^*|g) &= \sum_{u:u_1>u_2} f^*(u) \ln(f^*(u)) + \sum_{u:u_1\leq u_2} f^*(u) \ln(f^*(u)) \\
 &+ 2 \ln(M) \\
 &= \alpha \ln\left(\frac{2\alpha}{M(M-1)}\right) + (1-\alpha) \ln\left(\frac{2(1-\alpha)}{M(M+1)}\right) \\
 &+ 2 \ln(M). \tag{3.2.6}
 \end{aligned}$$

We can also consider the continuous version of (3.2.3), where  $g$  is the uniform density on the unit square and  $f$  a joint density that is absolutely continuous with respect to  $g$ :

$$f^* = \operatorname{argmin}_f I(f|g) = \operatorname{argmin}_f \int_{u \in [0,1]^2} f(u) \ln\left(\frac{f(u)}{g(u)}\right) du \tag{3.2.7}$$

Subject to:

$$\begin{aligned}
 \int_{u \in [0,1]^2} f(u) du &= 1 \\
 \int_{u \in [0,1]^2: u_1 > u_2} f(u) du &= \alpha \tag{3.2.8}
 \end{aligned}$$

**Proposition 3.2.2.** *The minimally informative distribution that satisfies 3.2.7 and 3.2.8 is equal to*

$$f^*(u_1, u_2) = \begin{cases} 2\alpha, & u_1 > u_2 \\ 2(1-\alpha), & u_1 \leq u_2 \\ (u_1, u_2) & \in [0, 1]^2 \end{cases} \tag{3.2.9}$$

*Proof.* Instead of considering the full class of joint densities that satisfies (3.2.8). Consider a joint density that is constant on both  $u_1 > u_2$  and  $u_1 \leq u_2$ :

$$f(u_1, u_2) = \begin{cases} 2\alpha, & u_1 > u_2 \\ 2(1-\alpha), & u_1 \leq u_2 \\ (u_1, u_2) & \in [0, 1]^2 \end{cases} \tag{3.2.10}$$

Let  $f^*$  be the minimal informative distribution solving to (3.2.7) and (3.2.8). We know that  $f^*$  is unique, because  $I(f|g)$  and the constraints are convex and has a global minimum. According to Kullback et al. [48] it follows that

$$\begin{aligned}
 I(f^*|g) &= \sup_{C \in \mathcal{C}} \sum_{i=1}^k P_{f^*}(C_i) \ln \left( \frac{P_{f^*}(C_i)}{P_g(C_i)} \right) \\
 P_f(C_i) &= \int_{C_i} f(x) dx
 \end{aligned} \tag{3.2.11}$$

where  $C = \bigcup_{i=1}^k C_i$  and  $\mathcal{C}$  is the set of all finite Borel partitions of  $[0, 1]^2$

We can write the constraints (3.2.8) in terms of a partition  $C = \{C_1, C_2\}$ , with

$$\begin{aligned}
 C_1 &= \{u_1 > u_2\} (u_1, u_2) \in [0, 1]^2 \\
 C_2 &= \{u_1 \leq u_2\} (u_1, u_2) \in [0, 1]^2
 \end{aligned} \tag{3.2.12}$$

giving

$$\begin{aligned}
 P_f(C_1) &= \alpha \\
 P_f(C_2) &= 1 - \alpha
 \end{aligned} \tag{3.2.13}$$

Because  $f^*$  is unique we must have

$$\begin{aligned}
 I(f|g) &\geq I(f^*|g) \geq \sum_{i=1}^2 P_{f^*}(C_i) \ln \left( \frac{P_{f^*}(C_i)}{P_g(C_i)} \right) \\
 &\geq I(f|g) \\
 &\Rightarrow f^* = f
 \end{aligned} \tag{3.2.14}$$

So  $f$  given by (3.2.10) is the solution to (3.2.7) and (3.2.8).  $\square$

The minimal relative information given of problem (3.2.7) given (3.2.10) is:

$$\begin{aligned}
 I(f^*|g) &= P_{f^*}(C_1) \ln \left( \frac{P_{f^*}(C_1)}{P_g(C_1)} \right) + P_{f^*}(C_2) \ln \left( \frac{P_{f^*}(C_2)}{P_g(C_2)} \right) \\
 &= \alpha \ln \left( \frac{\alpha}{\frac{1}{2}} \right) + (1 - \alpha) \ln \left( \frac{1 - \alpha}{\frac{1}{2}} \right) \\
 &= \alpha \ln(2\alpha) + (1 - \alpha) \ln(2(1 - \alpha))
 \end{aligned} \tag{3.2.15}$$

Likewise the means, variances, and correlation coefficient can be computed using this density which gives:

$$\begin{aligned}
E(u_1) &= \frac{1 + \alpha}{3} \\
E(u_2) &= \frac{2 - \alpha}{3} \\
Var(u_1) &= \frac{-2\alpha^2 + 2\alpha + 1}{18} \\
Var(u_2) &= \frac{-2\alpha^2 + 2\alpha + 1}{18} \\
Cor(u_1, u_2) &= \frac{4\alpha^2 - 4\alpha + 1}{-4\alpha^2 + 4\alpha + 2}.
\end{aligned} \tag{3.2.16}$$

Similarly we can compute the means, variances, and correlation coefficient with the solution of the discrete case.

The means, variances, and correlation of the utility values for  $a_1$  and  $a_2$  are computed using probability mass function  $f^*$  from proposition (3.2.1).

$$E_M(u_1) = \frac{M(1 + \alpha) + 2}{3M} \tag{3.2.17}$$

$$E_M(u_2) = \frac{M(2 - \alpha) + 1}{3M} \tag{3.2.18}$$

$$Var_M(u_1) = Var_M(u_2) = \frac{M^2(-2\alpha^2 + 2\alpha + 1) + M(2\alpha - 1) + 2}{18M^2} \tag{3.2.19}$$

$$Cor_M(u_1, u_2) = \frac{(M(2\alpha - 1) + 1)(M(2\alpha - 1) - 2)}{M^2(-4\alpha^2 + 4\alpha + 2) + M(2 - 4\alpha) - 4} \tag{3.2.20}$$

The limit of the minimal relative information as  $M$  approaches infinity is equal to

$$\lim_{M \rightarrow \infty} I(f^*|g) = \alpha \ln(2\alpha) + (1 - \alpha) \ln(2(1 - \alpha)). \tag{3.2.21}$$

Filling in the optimal probability mass function (3.2.1) into the relative information and then taking the limit as  $M$  approaches infinity gives the same result as (3.2.15).

As  $M$  approaches infinity the measures of  $u$  becomes

$$\begin{aligned}
\lim_{M \rightarrow \infty} E_M(u_1) &= \lim_{M \rightarrow \infty} \frac{M(1 + \alpha) + 2}{3M} \\
&= \lim_{M \rightarrow \infty} \frac{(1 + \alpha)}{3} + \frac{2}{3M} \\
&= \frac{1 + \alpha}{3}
\end{aligned} \tag{3.2.22}$$

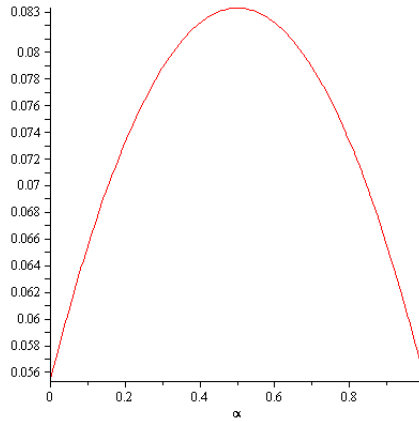
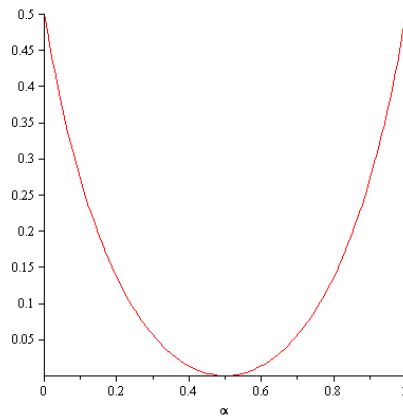
$$\begin{aligned}
 \lim_{M \rightarrow \infty} E_M(u_2) &= \lim_{M \rightarrow \infty} \frac{M(2-\alpha) + 1}{3M} \\
 &= \lim_{M \rightarrow \infty} \frac{(2-\alpha)}{3} + \frac{1}{3M} \\
 &= \frac{2-\alpha}{3}
 \end{aligned} \tag{3.2.23}$$

$$\begin{aligned}
 \lim_{M \rightarrow \infty} Var_M(u_1) &= \lim_{M \rightarrow \infty} \frac{M^2(-2\alpha^2 + 2\alpha + 1) + M(2\alpha - 1) + 2}{18M^2} \\
 &= \lim_{M \rightarrow \infty} \frac{(-2\alpha^2 + 2\alpha + 1)}{18} + \frac{(2\alpha - 1)}{18M} + \frac{-1}{18M^2} \\
 &= \frac{-2\alpha^2 + 2\alpha + 1}{18}
 \end{aligned} \tag{3.2.24}$$

$$\begin{aligned}
 \lim_{M \rightarrow \infty} Var_M(u_2) &= \lim_{M \rightarrow \infty} \frac{M^2(-2\alpha^2 + 2\alpha + 1) + M(2\alpha - 1) + 2}{18M^2} \\
 &= \lim_{M \rightarrow \infty} \frac{(-2\alpha^2 + 2\alpha + 1)}{18} + \frac{(2\alpha - 1)}{18M} + \frac{-1}{18M^2} \\
 &= \frac{-2\alpha^2 + 2\alpha + 1}{18}
 \end{aligned} \tag{3.2.25}$$

$$\begin{aligned}
 \lim_{M \rightarrow \infty} Cor_M(u_1, u_2) &= \lim_{M \rightarrow \infty} \frac{(M(2\alpha - 1) + 1)(M(2\alpha - 1) - 2)}{M^2(-4\alpha^2 + 4\alpha + 2) + M(2 - 4\alpha) - 4} \\
 &= \lim_{M \rightarrow \infty} \frac{M^2(4\alpha^2 - 4\alpha + 1)}{M^2(-4\alpha^2 + 4\alpha + 2) + M(2 - 4\alpha) - 4} \\
 &\quad + \frac{-M(2\alpha - 1)}{M^2(-4\alpha^2 + 4\alpha + 2) + M(2 - 4\alpha) - 4} \\
 &\quad + \frac{-2}{M^2(-4\alpha^2 + 4\alpha + 2) + M(2 - 4\alpha) - 4} \\
 &= \frac{4\alpha^2 - 4\alpha + 1}{-4\alpha^2 + 4\alpha + 2}.
 \end{aligned} \tag{3.2.26}$$

Figure 3.2.3 plots  $\alpha$  against the minimal relative information. As suspected no information is gained if  $\alpha = 0.5$ . Note that for  $\alpha = 0.5$  the correlation between the utility values of  $a_1, a_2$  are zero with mean and variance equal to the uniform distribution on  $[0, 1]$ .

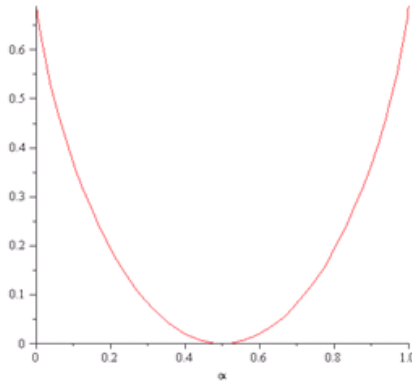
**Figure 3.2.1:** *Variance with respect to  $\alpha$* **Figure 3.2.2:** *Correlation with respect to  $\alpha$* 

### 3.2.2 $N$ Choice Alternatives

Let there be  $N$  choice alternatives  $a_1, a_2, \dots, a_N$ . Data is available of the form  $\mathcal{P}(u_i > u_j) = \alpha_{ij}, i \neq j, 0 \leq \alpha_{ij} \leq 1$  and we seek a minimum informative distribution over the utility values on a uniform hypercube  $\{\frac{1}{M}, \dots, 1\}^N$  which recovers the data.

The problem of finding such a distribution is:

**Figure 3.2.3:** Minimal relative information with respect to  $\alpha$



$$\begin{aligned}
 \operatorname{argmin}_f I(f|g) &= \operatorname{argmin}_f \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} f(u) \ln \left( \frac{f(u)}{g(u)} \right) \\
 &= \operatorname{argmin}_f \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} f(u) \ln(f(u)) + N \ln(M) \\
 g(u) &= \frac{1}{M^N}, \tag{3.2.27}
 \end{aligned}$$

subject to:

$$\begin{aligned}
 \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} f(u) &= 1 \\
 \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N : u_i > u_j} f(u) &= \alpha_{ij}, \forall i \neq j. \tag{3.2.28}
 \end{aligned}$$

We found no closed form solution for more than two choice variables nor were we able to find a solution using standard numerical algorithms. For standard numerical methods the number of unknown variables would be equal to  $M^N$ . Finding good numerical results using standard numerical methods becomes infeasible. However, the problem can be solved using more unconventional methods like IPF(Iterative Proportional Fitting) and PARFUM(PARAMeter Fitting for Uncertainty Models)[44, 16, 58, 13, 20, 17]. Kraan [39] shows that the PI problem is the dual of the convex optimization problem if the problem of finding a minimally informative distribution is feasible. Moreover the number of unk-

known values would be equal to the number of samples drawn, because the joint probability mass function can be written a vector of size  $K$ .

When the solution is feasible IPF is usually preferred over PARFUM, because of its fast convergence. However, if the problem is almost infeasible, the IPF solution may be 'peculiar'. The results of probabilistic inversion procedures can be found in sections 3.3.3 and 3.3.4 .

### 3.3 Minimal Relative Information Solution with a Standard Uniform Distribution Assuming Independence

The assumption of independence is often made without justification. Not only is this assumption mathematically convenient, but in many cases independence insures minimal information, since the independent distribution is the most entropic of all distributions with given margins. This section examines whether the independence assumptions common in modeling discrete choice data are information minimizing. We seek the minimally informative distributions recovering the paired comparisons data and satisfying independence constraints, and compare these with the solutions from the previous section. These comparisons can be found in sections 3.3.3, 3.3.4. It turns out that the independence constraint adds considerable information to the solution. Following the minimal information principle [35], dictates solutions without assuming independence should be preferred.

The minimum informative distribution over the choice alternatives assuming independence is :

$$f(u_1, \dots, u_N) = f_1(u_1) \times \dots \times f_N(u_N).$$

In the following subsection we derive the minimal joint distribution given paired comparison preferences and the independence assumption.

#### 3.3.1 Two Choice Alternatives

Let  $a_1$  and  $a_2$  be two choice alternatives with  $u_1$  independent of  $u_2$ . The probability that  $a_1$  is preferred over  $a_2$  is  $Q(a_1 \succ a_2) = \alpha$  and the probability mass functions over the utility values over  $a_1$  and  $a_2$  are given by  $f_1, f_2$ . The problem of finding a minimally informative distribution relative to the discrete uniform distribution on  $\{\frac{1}{M}, \dots, 1\}^2$  is:



$$\begin{aligned}
 \operatorname{argmin}_{f_1, f_2} I(f_1 f_2 | g) &= \operatorname{argmin}_{f_1, f_2} \sum_{u_1} \sum_{u_2} f_1(u_1) f_2(u_2) \ln \left( \frac{f_1(u_1) f_2(u_2)}{g} \right) \\
 &= \operatorname{argmin}_{f_1, f_2} \sum_{u_1} \sum_{u_2} f_1(u_1) f_2(u_2) \ln (f_1(u_1) f_2(u_2)) \\
 &+ 2 \ln(M), \tag{3.3.1}
 \end{aligned}$$

subject to:

$$\begin{aligned}
 \sum_{u_1} f_1(u_1) &= 1 \\
 \sum_{u_2} f_2(u_2) &= 1 \\
 \sum_{u_1} \sum_{u_1 > u_2} f_1(u_1) f_2(u_2) &= \alpha, \tag{3.3.2}
 \end{aligned}$$

with

$$0 \leq f_1(u_1), f_2(u_2) \leq 1.$$

**Proposition 3.3.1.** *The minimally informative solution of 3.3.1 and 3.3.2 satisfies the following two recurrence relationships*

$$\begin{aligned}
 f_1 \left( u_1 + \frac{1}{M} \right) &= f_1(u_1) e^{\lambda_{12} f_2(u_2 + \frac{1}{M})} \\
 f_2 \left( u_2 + \frac{1}{M} \right) &= f_2(u_2) e^{-\lambda_{12} f_1(u_1)} \tag{3.3.3}
 \end{aligned}$$

$$u_1, u_2 = \left\{ \frac{1}{M}, \dots, \frac{M-1}{M} \right\}$$

*Proof.* see appendix □

The problem now is to find  $f_1\left(\frac{1}{M}\right)$ ,  $f_2\left(\frac{1}{M}\right)$  and  $\lambda_{12}$  such that the constraints are met. This can be solved numerically. If a solution is found this would be unique, because the Lagrangian of this minimization problem (3.3.1) is convex. And convexity of the objective and constraint functions are sufficient conditions for a unique solution according to the Kuhn-Tucker Theorem. The relative information of the independent case is compared with a dependent case, which can be found in subsections 3.3.3 and 3.3.4.

### 3.3.2 $N$ Choice Alternatives

The problem of finding  $N$  independent utility values given  $\binom{N}{2}$  paired comparison constraints can be written as follow.

$$\begin{aligned}
 \operatorname{argmin}_{f_1, \dots, f_N} I(f_1 \dots f_N | g) &= \operatorname{argmin}_{f_1, \dots, f_N} \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} \prod_{i=1}^N f_i(u_i) \ln \left( \frac{\prod_{i=1}^N f_i(u_i)}{g(u)} \right) \\
 &= \operatorname{argmin}_{f_1, \dots, f_N} \sum_{u \in \{\frac{1}{M}, \dots, 1\}^N} \prod_{i=1}^N f_i(u_i) \ln \left( \prod_{i=1}^N f_i(u_i) \right) \\
 &\quad + N \ln(M), \tag{3.3.4}
 \end{aligned}$$

subject to:

$$\begin{aligned}
 \sum_{u_i} f_i(u_i) &= 1, \quad i = 1, \dots, N \\
 \sum_{u_i} \sum_{u_j > u_i} f_i(u_i) f_j(u_j) &= \alpha_{ij}, \quad i, j = 1, \dots, N, \quad i \neq j, \tag{3.3.5}
 \end{aligned}$$

with

$$\begin{aligned}
 0 &\leq f_1(u_1), \dots, f_N(u_N) \leq 1 \\
 u_i &= \left\{ \frac{1}{M}, \dots, 1 \right\}, \quad i = 1 \dots N.
 \end{aligned}$$

**Proposition 3.3.2.** *The minimally informative solution of 3.3.4 and 3.3.5 satisfies the following recurrence relationships*

$$\begin{aligned}
 f_1 \left( u_1 + \frac{1}{M} \right) &= f_1(u_1) e^{\sum_{j=2}^N \lambda_{1j} f_j(u_j + \frac{1}{M})} \\
 f_2 \left( u_2 + \frac{1}{M} \right) &= f_2(u_2) e^{-\lambda_{12} f_1(u_1) + \sum_{j=3}^N \lambda_{2j} f_j(u_j + \frac{1}{M})} \\
 \dots &= \dots \\
 \dots &= \dots \\
 \dots &= \dots \\
 f_N \left( u_N + \frac{1}{M} \right) &= f_N(u_N) e^{-\sum_{j=1}^{N-1} \lambda_{Nj} f_j(u_j + \frac{1}{M})} \tag{3.3.6}
 \end{aligned}$$

*Proof.* see appendix □

As with the case of two choice alternatives the problem is to find  $f_1(\frac{1}{M}), f_2(\frac{1}{M}), \dots, f_N(\frac{1}{M})$  and  $\lambda_{12}, \lambda_{13}, \dots, \lambda_{N(N-1)}$  such that the constraints are met with  $\lambda_{ij} = \lambda_{ji}$ .

### 3.3.3 Results Uniform distribution with Two Choice Alternatives

As mentioned above the problem can also be solved using probabilistic inversion techniques. Table 3.3.1 gives the results of sample based probabilistic inversion using IPF and table 3.3.2 shows the results of the asymptotic solution of the convex optimization problem (3.2.3).

**Table 3.3.1:** Probabilistic Inversion 50000 samples

Scenario	$\alpha$	$\mu_x$	$\mu_x$	$\sigma_x$	$\sigma_y$	$\rho_{xy}$	$I(f u^2)$
1	0.50	0.5015	0.4997	0.2893	0.2877	0.0065	0.0000
2	0.60	0.4669	0.5323	0.2879	0.2865	0.0095	0.0199
3	0.70	0.4362	0.5666	0.2819	0.2818	0.0573	0.0818
4	0.80	0.4021	0.5979	0.2715	0.2696	0.1358	0.1920
5	0.90	0.3673	0.6332	0.2578	0.2553	0.2653	0.3670
6	0.95	0.3497	0.6507	0.2468	0.2454	0.3626	0.4935
7	0.99	0.3392	0.6642	0.2395	0.2370	0.4645	0.6360

**Table 3.3.2:** Asymptotic solution

Scenario	$\alpha$	$\mu_x$	$\mu_x$	$\sigma_x$	$\sigma_y$	$\rho_{xy}$	$I(f u^2)$
1	0.50	0.5000	0.5000	0.2887	0.2887	0.0000	0.0000
2	0.60	0.4667	0.5333	0.2867	0.2867	0.0135	0.0201
3	0.70	0.4333	0.5667	0.2809	0.2809	0.0563	0.0823
4	0.80	0.4000	0.6000	0.2708	0.2708	0.1364	0.1927
5	0.90	0.3667	0.6333	0.2560	0.2560	0.2712	0.3681
6	0.95	0.3500	0.6500	0.2466	0.2466	0.3699	0.4946
7	0.99	0.3367	0.6633	0.2380	0.2380	0.4709	0.6371

From tables 3.3.1 and 3.3.2 it follows that the probabilistic inversion solution is close to the asymptotic solution.

Table 3.3.3 below shows the results of adding the independence constraint to the problem.

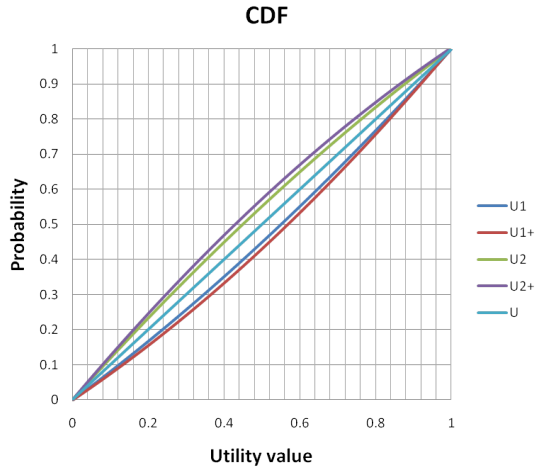
**Table 3.3.3:** Results with Independence Constraints

Scenario	$\alpha$	$\mu_1$	$\mu_2$	$\sigma_1^2$	$\sigma_2^2$	$I(f u^2)$
1	0.50	0.505	0.514	0.079	0.079	0.000
2	0.60	0.455	0.564	0.075	0.090	0.036
3	0.70	0.405	0.614	0.068	0.115	0.135
4	0.80	0.356	0.662	0.056	0.153	0.308
5	0.90	0.300	0.711	0.037	0.212	0.565
6	0.95	0.297	0.738	0.036	0.222	0.690

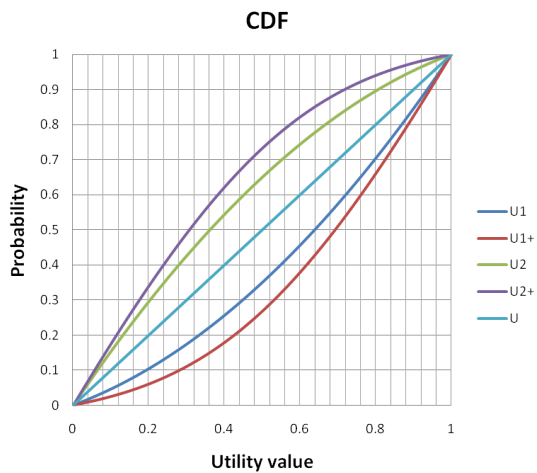
From table 3.3.4 it follows that information score of the solution with the independence constraints is higher than the solution without the independence constraint with equality when  $\alpha = 0.5$ . The effect of the higher information score can also be seen from the cumulative probability distribution function (CDF), see

figures 3.3.1,3.3.2. The marginal CDF's of  $u_1, u_2$  without independence marked by  $U1, U2$  are closer to the starting distribution  $g$  which is the standard uniform distribution than the marginal CDF's of  $u_1, u2$  with independence marked by  $U1+, U2+$ .

**Figure 3.3.1:** CDF's of  $u_1, u_2$  with and without independence for  $\alpha = 0.6$



**Figure 3.3.2:** CDF's of  $u_1, u_2$  with and without independence for  $\alpha = 0.8$



**Table 3.3.4:** Comparison between Dependent and Independent Case

Scenario	Dependent	Independent	$\frac{I_{independent} - I_{dependent}}{I_{dependent}} \times 100\%$
1	0.0000	0.0000	0.00%
2	0.0201	0.0360	79.1%
3	0.0823	0.1350	64.0%
4	0.1927	0.3080	59.8%
5	0.3680	0.5650	53.5%
6	0.4946	0.6900	39.5%

### 3.3.4 Results Uniform distribution with Three Choice Alternatives

Table 3.3.5 shows paired comparisons scenarios for three choice alternatives. Table 3.3.6 and 3.3.7 give the result for the solution using probabilistic inversion and constraint optimization, respectively. As expected the information score for the solution without assuming independence is as least as small as the one with the independence assumption see table 3.3.8.

**Table 3.3.5:** Scenarios Marginal Constraints

Scenario	$\alpha_{12}$	$\alpha_{13}$	$\alpha_{23}$
1	0.8	0.54	0.31
2	0.5	0.5	0.5
3	0.6	0.35	0.71

**Table 3.3.6:** Solution with Probabilistic Inversion and 100000 samples

Scenario	$\mu_1$	$\mu_2$	$\mu_3$	$\sigma_1^2$	$\sigma_2^2$	$\sigma_3^2$	$\rho_{12}$	$\rho_{13}$	$\rho_{23}$	$I(f u^3)$
1	0.59	0.38	0.54	0.08	0.07	0.08	0.01	0.01	0.03	0.21
2	0.5	0.50	0.50	0.08	0.08	0.084	0.00	0.0	0	0
3	0.49	0.53	0.49	0.08	0.08	0.081	-0.05	0.00	0.05	0.53

**Table 3.3.7:** Solution Recurrence Relations

Scenario	$\alpha_{12}$	$\alpha_{13}$	$\alpha_{23}$	$\mu_1$	$\mu_2$	$\mu_3$	$\sigma_1^2$	$\sigma_2^2$	$\sigma_3^2$
1	0.800	0.540	0.310	0.589	0.335	0.583	0.044	0.110	0.106
2	0.500	0.500	0.500	0.502	0.506	0.508	0.080	0.082	0.081
3	0.600	0.350	0.710	0.452	0.525	0.508	0.128	0.113	0.014

**Table 3.3.8:** Comparison Dependent and Independent Case

Scenario	Dependent	Independent	$\frac{I_{independent} - I_{dependent}}{I_{dependent}} \times 100\%$
1	0.208	0.545	162%
2	0	0	0%
3	0.119	0.211	77%

### 3.4 Normal distribution : Probit model

Thurstone formulated the *Law of Comparative Judgment* to elicit a distribution over the utility values of the alternatives based on the preferences of one or more individuals. The law formulates a model that is not solvable in its general form; various restrictions are imposed to ensure solvability. The law of comparative judgment assumes that the value  $u(a_i)$  is normally distributed with mean  $\mu_i$  and standard deviation  $\sigma_i$ . The difference between two alternatives  $a_i$  and  $a_j$  is again normally distributed with mean  $\mu_{ij} = \mu_i - \mu_j$  and standard deviation  $\sigma_{ij} = \sqrt{\sigma_i^2 + \sigma_j^2 - 2\rho_{ij}\sigma_i\sigma_j}$ . Where  $\rho_{ij}$  is the correlation coefficient of the utility values from alternative  $a_i$  and  $a_j$ .

In our next examples we want to seek a minimally informative distribution relative to the standard normal distribution. Finding a generic distribution that is minimal with respect to the standard normal is rather complex. To enhance comparison with standard results, we seek minimally informative distributions within the set of joint normal distributions. Thus, it suffices to find the parameters  $\bar{\mu}$  and  $\Sigma$  such that the joint normal distribution with these parameters is minimally informative with respect to the standard normal distribution.

Thurstone proposed three different models, known as Thurstone A, Thurstone B, and Thurstone C to find a distribution over utility values that satisfies the marginal constraints from stakeholder data. Thurstone A model assumes that the correlation term is constant, with varying means and standard deviations. Thurstone B model assumes that the correlation is zero and the standard deviations vary. Thurstone C model assumes that the correlation is zero and constant standard deviation, often equal to one. By formulating the problem as a problem of minimal relative information we will derive solutions that obey the Thurstone B assumption of zero correlation, varying means and standard deviation. We have obtained the solution without assuming any dependency structure of the minimally informative distribution. We will show that the solution that follows from the Thurstone C assumption adds more information to the problem than necessary.

#### 3.4.1 Minimal Information Solution for Two Alternatives

The relative information between two multivariate normal distributions  $f$  and  $g$  is given by Whittaker and Robinson [99]:

$$\begin{aligned}
I(f|g) &= \frac{1}{2} [\bar{\mu}_f - \bar{\mu}_g, \Sigma_g^{-1} (\bar{\mu}_f - \bar{\mu}_g)] + \frac{1}{2} \text{tr} (\Sigma_f \Sigma_g^{-1}) \\
&- \frac{1}{2} \ln (|\Sigma_f \Sigma_g^{-1}|) - \frac{N}{2},
\end{aligned} \tag{3.4.1}$$

with  $f : \bar{X} \sim M(\bar{\mu}_f, \Sigma_f)$  and  $g : \bar{X} \sim M(\bar{\mu}_g, \Sigma_g)$ .

In our case  $g$  is multivariate standard normal so the relative information becomes

$$I(f|g) = \frac{1}{2} [\bar{\mu}_f, \bar{\mu}_f] + \frac{1}{2} \text{tr} (\Sigma_f) - \frac{1}{2} \ln (|\Sigma_f|) - \frac{N}{2} \tag{3.4.2}$$

We will first look at the bivariate case. We want to find  $\bar{\mu}_f = (\mu_1, \mu_2)$  and  $\Sigma_f = (\sigma_1, \sigma_2, \rho)$  with the constraint

$$\mathcal{P}(u_1 > u_2) = \alpha,$$

that minimizes (3.4.2). We can rewrite the equation to obtain:

$$\begin{aligned}
\mathcal{P}(u_1 > u_2) &= \mathcal{P}(u_1 - u_2 > 0) \\
&= \mathcal{P}(u_1 - u_2 - \mu_{12} > -\mu_{12}) \\
&= \mathcal{P}\left(\frac{u_1 - u_2 - \mu_{12}}{\sigma_{12}} > \frac{-\mu_{12}}{\sigma_{12}}\right) \\
&= \mathcal{P}\left(\bar{X} > \frac{-\mu_{12}}{\sigma_{12}}\right) \\
&= \mathcal{P}\left(\bar{X} < \frac{\mu_{12}}{\sigma_{12}}\right) \\
&= \Phi\left(\frac{\mu_{12}}{\sigma_{12}}\right) = \alpha
\end{aligned} \tag{3.4.3}$$

where  $\mu_{12} = \mu_1 - \mu_2$ ,  $\sigma_{12} = \sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2\sigma_1\sigma_2}$  and  $\Phi$  the cumulative standard normal distribution. Taking the inverse distribution over the constraint gives

$$\frac{\mu_1 - \mu_2}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2\sigma_1\sigma_2}} = \Phi^{-1}(\alpha). \tag{3.4.4}$$

The minimization problem can be formulated as follows

$$\underset{\bar{\mu}_f, \Sigma_f}{\text{argmin}} I(f|g) = \underset{\bar{\mu}_f, \Sigma_f}{\text{argmin}} \frac{1}{2} (\mu_1^2 + \mu_2^2) + \frac{1}{2} (\sigma_1^2 + \sigma_2^2) - \frac{1}{2} \ln (\sigma_1^2 \sigma_2^2 - \rho^2 \sigma_1^2 \sigma_2^2) - 1, \tag{3.4.5}$$

subject to:

$$\frac{\mu_1 - \mu_2}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2\sigma_1\sigma_2}} = \Phi^{-1}(\alpha). \tag{3.4.6}$$

**Proposition 3.4.1.** *The minimal informative solution to 3.4.5 and 3.4.6 is given by*

$$\begin{aligned}\mu_1^* &= \delta \sqrt{\frac{1}{2 + \delta^2}}, \mu_2^* = -\delta \sqrt{\frac{1}{2 + \delta^2}} \\ \sigma_1^* &= \sqrt{\frac{2}{2 + \delta^2}}, \sigma_2^* = \sqrt{\frac{2}{2 + \delta^2}}, \rho^* = 0 \\ \delta &= \Phi^{-1}(\alpha)\end{aligned}$$

*Proof.* See Appendix. □

**Proposition 3.4.2.** *The minimal value for  $I(f|g)$  given in proposition 3.4.1 is*

$$I(f^*|g) = \ln\left(\frac{2 + \delta^2}{2}\right)$$

*Proof.* Substitute the values of  $\mu_1^*, \mu_2^*, \sigma_1^*, \sigma_2^*, \rho^*$  into  $I(f^*|g)$  □

The Thurstone models are usually solved using least squares instead of minimal relative information. In case of Thurstone C (unit variance, zero correlation) the formulation is:

$$\operatorname{argmin}_{\mu_1, \mu_2} \left( \mu_1 - \mu_2 - \delta\sqrt{2} \right)^2 \quad (3.4.7)$$

with  $\delta = \Phi^{-1}(\alpha)$ .

Equation 3.4.7 has a trivial solution namely  $\mu_1^* = \frac{1}{2}\sqrt{2}\delta$  and  $\mu_2^* = -\frac{1}{2}\sqrt{2}\delta$ , which gives  $\mu_1^* + \mu_2^* = 0$ . In general it follows that for the optimal solution

$$\sum_{i=1}^N \mu_i = 0.$$

**Proposition 3.4.3.** *The minimally informative solution to 3.4.5 and 3.4.6 according to Thurstone C is  $\mu_1^* = \frac{1}{2}\sqrt{2}\delta$  and  $\mu_2^* = -\frac{1}{2}\sqrt{2}\delta$*

*Proof.* The minimally informative solution according to equation 3.4.2 according to Thurstone C (unit variance, zero correlation) is

$$\begin{aligned}\operatorname{argmin}_f I(f|g) &= \operatorname{argmin}_{\mu_1, \mu_2} \frac{1}{2} (\mu_1^2 + \mu_2^2) + \frac{1}{2} (1 + 1) - \frac{1}{2} \ln(1) - 1 \\ &= \operatorname{argmin}_{\mu_1, \mu_2} \frac{1}{2} (\mu_1^2 + \mu_2^2),\end{aligned} \quad (3.4.8)$$



subject to

$$\mu_1 - \mu_2 = \delta\sqrt{2} \quad (3.4.9)$$

The Lagrangian is

$$\mathcal{L}(\mu_1, \mu_2, \lambda) = \frac{1}{2}(\mu_1^2 + \mu_2^2) + \lambda_{12}(\mu_1 - \mu_2 - \delta\sqrt{2}) \quad (3.4.10)$$

and the derivatives of the Lagrangian are

$$\begin{aligned} \frac{\partial L}{\partial \mu_1} &= \mu_1 + \lambda \\ \frac{\partial L}{\partial \mu_2} &= \mu_2 - \lambda \\ \frac{\partial L}{\partial \lambda} &= \mu_1 - \mu_2 - \delta\sqrt{2} \end{aligned}$$

setting the derivatives to zero yields

$$\begin{aligned} \mu_1^* &= \frac{1}{2}\sqrt{2}\delta \\ \mu_2^* &= -\frac{1}{2}\sqrt{2}\delta \\ \lambda^* &= \frac{1}{2}\sqrt{2}\delta \end{aligned}$$

□

It follows from proposition 3.4.3 that the same solution is obtained from either solving (3.4.7) or (3.4.8),(3.4.9) .

**Proposition 3.4.4.** *The relative information of the Thurstone C solution ( $T_C$ ) is given by:*

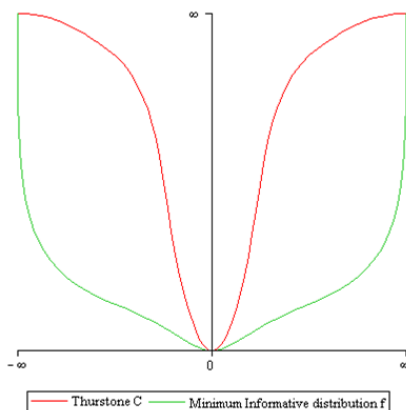
$$I(T_C|g) = \frac{1}{2}\delta^2 \quad (3.4.11)$$

*Proof.* Filling in the optimal solution from proposition 3.4.3 into 3.4.8 gives

$$I(T_C|g) = \frac{1}{2}\delta^2$$

□

From proposition 3.4.1 and 3.4.2 it follows that

**Figure 3.4.1:** Minimal relative information of Thurstone C and  $f^*$  with respect to  $\delta$ 

$$\begin{aligned}
 I(T_C|g) &\geq I(f^*|g) \\
 \frac{1}{2}\delta^2 &\geq \ln\left(1 + \frac{\delta^2}{2}\right)
 \end{aligned} \tag{3.4.12}$$

with equality when  $\delta = 0$  or  $\alpha = 0.5$ .

In the two dimensional case it can be concluded that the Thurstone C solution is more informative than the one obtained by minimizing the relative information with respect to the given constraint.

The reason that the Thurstone C solution does not satisfy the constraints for  $\alpha \neq 0.5$  is that the variance is assumed to be one, so that the contribution of the tails of the normal distributions becomes large.

### 3.4.2 Minimal Information Solution for Three Alternatives

In this section we will find the minimally informative distribution with respect to the standard normal distribution for three choice alternatives.

The relative information is given by

$$\begin{aligned}
 I(f|g) &= \frac{1}{2}(\mu_1^2 + \mu_2^2 + \mu_3^2) + \frac{1}{2}(\sigma_1^2 + \sigma_2^2 + \sigma_3^2) \\
 &\quad - \frac{1}{2}\ln(\sigma_1^2\sigma_2^2\sigma_3^2\{1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}\}) - \frac{3}{2}.
 \end{aligned} \tag{3.4.13}$$

We want to minimize the relative information subject to the following constraints

$$\begin{aligned}
\frac{\mu_1 - \mu_2}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho_{12}^2\sigma_1\sigma_2}} &= \Phi^{-1}(\alpha_{12}) = \delta_{12} \\
\frac{\mu_2 - \mu_3}{\sqrt{\sigma_2^2 + \sigma_3^2 - 2\rho_{23}^2\sigma_2\sigma_3}} &= \Phi^{-1}(\alpha_{23}) = \delta_{23} \\
\frac{\mu_3 - \mu_1}{\sqrt{\sigma_3^2 + \sigma_1^2 - 2\rho_{31}^2\sigma_3\sigma_1}} &= \Phi^{-1}(\alpha_{31}) = \delta_{31}.
\end{aligned} \tag{3.4.14}$$

A closed form solution for (3.4.13) and (3.4.14) has not been found, but we can look at the set of feasible solutions. We did however solve the problem numerically using the feasible set of solutions. The set of feasible solution is obtained by looking at the constraints (3.4.14) and setting the partial derivatives with respect to the  $\mu$ 's,  $\sigma$ 's and  $\rho$ 's of the Lagrangian to zero. Investigating (3.4.14) gives the following proposition 3.4.5.

**Proposition 3.4.5.** *There is no solution to (3.4.13) and (3.4.14) if  $\delta_{12}, \delta_{23}, \delta_{31} > 0$  or  $\delta_{12}, \delta_{23}, \delta_{31} < 0$ .*

*Proof.* Let  $\sigma_{ij} = \sqrt{\sigma_i^2 + \sigma_j^2 - 2\rho_{ij}^2\sigma_i\sigma_j} > 0$  and  $\delta_{ij} > 0$ . Then the three constraints from (3.4.14) become

$$\begin{aligned}
\mu_1 - \mu_2 &= \sigma_{12}\delta_{12} \\
\mu_2 - \mu_3 &= \sigma_{23}\delta_{23} \\
\mu_3 - \mu_1 &= \sigma_{31}\delta_{31}.
\end{aligned} \tag{3.4.15}$$

Summing up the first two equations of (3.4.15)

$$\mu_1 - \mu_3 = \sigma_{12}\delta_{12} + \sigma_{23}\delta_{23}. \tag{3.4.16}$$

And multiplying the last equation of (3.4.15):

$$\mu_1 - \mu_3 = -\sigma_{31}\delta_{31}. \tag{3.4.17}$$

From (3.4.16) it follows that

$$\mu_1 - \mu_3 > 0 \tag{3.4.18}$$

And from (3.4.17) it follows that

$$\mu_1 - \mu_3 < 0 \tag{3.4.19}$$

given  $\delta_{12}, \delta_{23}, \delta_{31} > 0$  and  $\sigma_{ij} > 0$ . Hence there is no solution. The same is true if  $\delta_{12}, \delta_{23}, \delta_{31} < 0$

□

The partial derivatives of the Lagrangian from (3.4.13) and (3.4.14) with respect to each of the variables are:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \mu_i} &= \mu_i + \sum_{j \neq i} \frac{(2 * 1_{\{j > i\}} - 1) \lambda_{ij}}{\sqrt{\langle \bar{\sigma}_{ij}, R_{(ij)} \bar{\sigma}_{ij} \rangle}} \\
\frac{\partial \mathcal{L}}{\partial \sigma_i} &= \sigma_i - \frac{1}{\sigma_i} - \sum_{j \neq i} \frac{\lambda_{ij} (\mu_i - \mu_j) (\sigma_i - \rho_{ij}^2 \sigma_j)}{\langle \bar{\sigma}_{ij}, R_{(ij)} \bar{\sigma}_{ij} \rangle^{\frac{3}{2}}} \\
\frac{\partial \mathcal{L}}{\partial \rho_{ij}} &= \frac{1}{2} (C_{ij}^{-1} + C_{ji}^{-1}) + \frac{2 \lambda_{ij} (\mu_i - \mu_j) \rho_{ij} \sigma_i \sigma_j}{\langle \bar{\sigma}_{ij}, R_{(ij)} \bar{\sigma}_{ij} \rangle^{\frac{3}{2}}} \\
\frac{\partial \mathcal{L}}{\partial \lambda_{ij}} &= \frac{\mu_i - \mu_j}{\sqrt{\sigma_i^2 + \sigma_j^2 - 2 \rho_{ij}^2 \sigma_i \sigma_j}} - \delta_{ij}
\end{aligned} \tag{3.4.20}$$

with

$$\bar{\sigma}_{ij} = (\sigma_i, \sigma_j)$$

$$R_{(ij)} = \begin{pmatrix} 1 & -\rho_{ij}^2 \\ -\rho_{ij}^2 & 1 \end{pmatrix}$$

$$(\lambda_{ij} = \lambda_{ji})$$

$$(\rho_{ij} = \rho_{ji})$$

Setting

$$\frac{\partial \mathcal{L}}{\partial \mu_i} = \mu_i + \sum_{j \neq i} \frac{(2 * 1_{\{j > i\}} - 1) \lambda_{ij}}{\sqrt{\langle \bar{\sigma}_{ij}, R_{(ij)} \bar{\sigma}_{ij} \rangle}}$$

to zero it follows that

$$\sum_{i=1}^M \mu_i = 0$$

The feasible solutions of  $\rho$ 's are given by  $1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23} > 0$ . We can directly note that for  $\rho_{12} = \rho_{13} = \rho_{23} = 0$  the relative information is minimal, because then the term  $\ln(1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23})$  becomes zero. The minimal solution will consist solely out of varying  $\mu$ 's and  $\sigma$ 's.

In view of (3.4.15) the feasible set of solution with constant variance and constant correlation satisfy

$$\delta_{12} + \delta_{23} = \delta_{13}. \quad (3.4.21)$$

Equation 3.4.21 looks familiar to the inequality formulated by Marschak [57]. His constraint for the existence of a distribution over utility for three choice alternatives is given by equation (3.4.22)

$$\alpha_{12} + \alpha_{23} \geq \alpha_{13} \quad (3.4.22)$$

The feasible set for varying means and standard deviation with zero correlation is larger than the set with varying mean, constant variance, and varying correlation. A number of scenarios for  $\delta_{ij}$  is worked out and solved in following subsection.

### 3.4.3 Results Normal distribution with Three Choice Alternatives

The scenarios for the marginal constraints to the problem of finding a minimally informative solution using a normal starting distribution is given by table 3.4.1. Table 3.4.2 shows the result for varying means and variances and zero correlation. Table 3.4.3 shows the result for constant variance. We also give the solution for the Thurstone *B* and *C* solution in tables 3.4.4 and 3.4.5. In a number of cases the information score for the Thurstone *B* and *C* solution are smaller than the information score for the minimally informative solution, but the Thurstone *B* and *C* solution do not satisfy the marginal constraint.

**Table 3.4.1:** *Scenarios Marginal Constraints*

Scenario	$\alpha_{12}$	$\alpha_{23}$	$\alpha_{31}$
1	0.8	0.31	0.4
2	0.6	0.7	0.3
3	0.4	0.7	0.2
4	0.4	0.3	0.8
5	0.5	0.5	0.5

$\Delta_{\text{Thur. B}}$  and  $\Delta_{\text{Thur. C}}$  respectively are the sum of squared difference between the probabilities  $\alpha_{ij}$  provided and  $\alpha'_{ij}$  obtained.

**Table 3.4.2:** Results Minimal Informative Distribution  $f^*$ 

Scenario	$\mu_1$	$\mu_2$	$\mu_3$	$\sigma_1$	$\sigma_2$	$\sigma_3$
1	0.4457	-0.5534	0.1077	0.8401	0.8387	1.0364
2	0.3969	0.0204	-0.4173	1.4005	0.4973	0.6702
3	0.1642	0.4969	-0.6611	0.6295	1.1522	0.7519
4	-0.4513	-0.1177	0.569	0.8626	0.9946	0.8517
5	0	0	0	1	1	1

**Table 3.4.3:** Results Minimal Informative Distribution  $f^*$  with constant variance and non-zero correlation

Scenario	$\mu_1$	$\mu_2$	$\mu_3$	$\sigma$	$\rho_{12}$	$\rho_{23}$	$\rho_{31}$
1	0.4326	-0.5372	0.1046	0.9153	0.4566	0	0
2	0.3509	0.008	-0.3589	0.9570	0	0.8560	0
3	0.1413	0.4619	-0.6032	0.8949	0	0	0.7151
4	-0.4419	-0.1162	0.5581	0.9091	0	0	0.3821
5	0	0	0	1	0	0	0

**Table 3.4.4:** Results Thurstone B Model

Scenario	$\mu_1$	$\mu_2$	$\mu_3$	$\sigma_1$	$\sigma_2$	$\sigma_3$
1	0.0056	-0.0503	0.1035	0.0917	0.4856	2.4227
2	0.2302	0.0213	-0.1614	1.6799	0.4466	0.8735
3	0.0715	0.1550	-0.1687	1.4961	0.8032	0.7007
4	N/A	N/A	N/A	N/A	N/A	N/A
5	N/A	N/A	N/A	N/A	N/A	N/A

**Table 3.4.5:** Results Thurstone C Model

Scenario	$\mu_1$	$\mu_2$	$\mu_3$	$\sigma_1$	$\sigma_2$	$\sigma_3$
1	0.1630	-0.2773	0.1143	1	1	1
2	0.3666	0.1278	-0.4944	1	1	1
3	0.1278	0.5162	-0.6439	1	1	1
4	-0.3666	-0.2773	0.6439	1	1	1
5	0	0	0	1	1	1

**Table 3.4.6:** Recovery of Marginal Constraints

Scenario	$I_I$	$I_{II}$	$I_{\text{Thur. C}}$	$I_{\text{Thur. B}}$	$\Delta_{\text{Mininf}}$	$\Delta_{\text{Thur. C}}$	$\Delta_{\text{Thur. B}}$
1	0.314	0.381	0.058	3.790	0	0.226	0.315
2	0.757	0.792	0.198	0.855	0	0.431	0.313
3	1.134		0.349	0.388	0	0.516	0.376
4	0.314	0.365	0.313	5.132	0	0.569	0.386
5	0	0	0	N/A	0	0	N/A

- $I_I$  - Relative information from the solution of (3.4.13) and (3.4.14) with zero correlation 3.4.2
- $I_{II}$  - Relative information from solution of (3.4.13) and (3.4.14) with constant variance and non-zero correlation 3.4.3
- $I_{\text{Thur. C}}$  - Relative information from the Thurstone C case
- $I_{\text{Thur. B}}$  - Relative information from the Thurstone B case

## 3.5 Appendix

### Derivation Minimal Informative Distribution over Two Choice Alternatives and Uniform Starting Distribution

The general Lagrange function  $\mathcal{L} : \mathbb{R}^{n+m} \rightarrow \mathbb{R}$  is defined as,

$$\mathcal{L}(x, \lambda) = q(x) + \lambda^T r(x),$$

where  $m$  is the number of constraint functions and  $n$  the number of variables and  $q(x)$  the objective function. Extreme values can be found by setting the gradients of  $x$  and  $\lambda$  equal to zero. The objective function  $I(f|g)$  can be simplified by using the probability mass function of  $g$ .

$$\begin{aligned} I(f|g) &= \sum_{u_1=\frac{1}{M}}^1 \sum_{u_2=\frac{1}{M}}^1 f(u_1, u_2) \ln \left( \frac{f(u_1, u_2)}{g(u_1, u_2)} \right) \\ &= \sum_{u_1=\frac{1}{M}}^1 \sum_{u_2=\frac{1}{M}}^1 f(u_1, u_2) \ln(f(u_1, u_2)) + 2 \ln(M). \end{aligned} \quad (3.5.1)$$

The gradient with respect to  $f(u_1, u_2)$  is given by

$$\frac{\partial \mathcal{L}}{\partial f(u_1, u_2)} = \ln(f(u_1, u_2)) + 1 + \lambda_1 + \lambda_{12} 1_{\{u_1 > u_2\}}. \quad (3.5.2)$$

Likewise the gradients for  $\lambda_1$  and  $\lambda_{12}$  are given by

$$\frac{\partial \mathcal{L}}{\partial \lambda_1} = \sum_{u_1} \sum_{u_2} f(u_1, u_2) - 1 \quad (3.5.3)$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{12}} = \sum_{u_1} \sum_{u_1 > u_2} f(u_1, u_2) - \alpha. \quad (3.5.4)$$

Setting the gradient of  $f(u_1, u_2)$  to zero gives

$$f(u_1, u_2) = e^{-(1+\lambda_1+\lambda_{12}1_{\{u_1 > u_2\}})}. \quad (3.5.5)$$

Setting the gradients of  $\lambda_1$  and  $\lambda_{12}$  to zero and substituting  $f(u_1, u_2)$  gives

$$\frac{\partial \mathcal{L}}{\partial \lambda_1} = \frac{M(M-1)}{2} e^{-(1+\lambda_1+\lambda_{12})} + \frac{M(M+1)}{2} e^{-(1+\lambda_1)} - 1 = 0 \quad (3.5.6)$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_{12}} = \frac{M(M-1)}{2} e^{-(1+\lambda_1+\lambda_{12})} - \alpha = 0. \quad (3.5.7)$$

After substituting it follows that the distribution  $f(u_1, u_2)$  that minimizes the relative information with the given constraints is equal to:

$$f^*(u_1, u_2) = \begin{cases} \frac{2\alpha}{M(M-1)}, & u_1 > u_2 \\ \frac{2(1-\alpha)}{M(M+1)}, & u_1 \leq u_2 \end{cases}. \quad (3.5.8)$$

## Derivation Minimal Informative Distribution over Two Choice Alternatives and with Independent Uniform Marginals

The problem of finding a minimally informative distribution relative to the discrete uniform distribution on the unit square discretized by  $\{\frac{1}{M}, \dots, 1\}^2$  can be formulated as follow:

$$\begin{aligned} \operatorname{argmin}_{f_1, f_2} I(f_1, f_2 | g) &= \operatorname{argmin}_{f_1, f_2} \sum_{u_1=\frac{1}{M}}^1 \sum_{u_2=\frac{1}{M}}^1 f_1(u_1) f_2(u_2) \ln \left( \frac{f_1(u_1) f_2(u_2)}{g(u_1, u_2)} \right) \\ &= \operatorname{argmin}_{f_1, f_2} \sum_{u_1=\frac{1}{M}}^1 \sum_{u_2=\frac{1}{M}}^1 f_1(u_1) f_2(u_2) \ln (f_1(u_1) f_2(u_2)) \\ &+ 2 \ln(M), \end{aligned} \quad (3.5.9)$$



Subject to:

$$\begin{aligned} \sum_{u_1=\frac{1}{M}}^1 f_1(u_1) &= 1 \\ \sum_{u_2=\frac{1}{M}}^1 f_2(u_2) &= 1 \\ \sum_{u_1=\frac{1}{M}}^1 \sum_{u_1>u_2}^1 f_1(u_1) f_2(u_2) &= \alpha, \end{aligned} \quad (3.5.10)$$

with

$$0 \leq f_1(u_1), f_2(u_2) \leq 1$$

The gradient of  $f_1(u_1)$ ,  $u_1 = \{\frac{1}{M} \dots 1\}$  is equal to:

$$\frac{\partial L}{\partial f_1(u_1)} = \sum_{u_2=\frac{1}{M}}^1 f_2(u_2) [\ln(f_1(u_1) f_2(u_2)) + 1] + \lambda_1 + \lambda_{12} \sum_{u_2=u_1+\frac{1}{M}}^1 f_2(u_2). \quad (3.5.11)$$

And the gradient of  $f_2(u_2)$ ,  $u_2 = \{\frac{1}{M} \dots 1\}$  is equal to:

$$\frac{\partial L}{\partial f_2(u_2)} = \sum_{u_1=\frac{1}{M}}^1 f_1(u_1) [\ln(f_1(u_1) f_2(u_2)) + 1] + \lambda_2 + \lambda_{12} \sum_{u_1=\frac{1}{M}}^{u_2-\frac{1}{M}} f_1(u_1). \quad (3.5.12)$$

Putting the gradients equal to zero gives a system of non-linear equations

$$\begin{aligned} \ln(f_1(u_1)) + \sum_{u_2=\frac{1}{M}}^1 f_2(u_2) \ln(f_2(u_2)) + 1 + \lambda_1 + \lambda_{12} \sum_{u_2=u_1+\frac{1}{M}}^1 f_2(u_2) &= 0 \\ \ln(f_2(u_2)) + \sum_{u_1=\frac{1}{M}}^1 f_1(u_1) \ln(f_1(u_1)) + 1 + \lambda_2 + \lambda_{12} \sum_{u_1=\frac{1}{M}}^{u_2-\frac{1}{M}} f_1(u_1) &= 0 \end{aligned} \quad (3.5.13)$$

which leads to two recurrence relations that are .

$$\begin{aligned} f_1\left(u_1 + \frac{1}{M}\right) &= f_1(u_1) e^{\lambda_{12} f_2(u_2 + \frac{1}{M})} \\ f_2\left(u_2 + \frac{1}{M}\right) &= f_2(u_2) e^{-\lambda_{12} f_1(u_1)}, \end{aligned} \quad (3.5.14)$$

for  $u_1, u_2 = \left\{ \frac{1}{M}, \dots, \frac{M-1}{M} \right\}$ . The problem now is to find values for  $f_1 \left( \frac{1}{M} \right)$ ,  $f_2 \left( \frac{1}{M} \right)$ ,  $\lambda_{12}$  such that the constraints are met.

## Derivation Minimal Informative Distribution over $N$ Choice Alternatives and with Independent Uniform Marginals

Then problem of finding a minimally informative distribution relative to the discrete uniform distribution on the unit hypercube  $\left\{ \frac{1}{M}, \dots, 1 \right\}^N$  given  $\binom{N}{2}$  paired comparison constraints can be written as follow:

$$\begin{aligned} \operatorname{argmin}_{f_1, \dots, f_N} I(f_1 \dots f_N | g) &= \operatorname{argmin}_{f_1, \dots, f_N} \sum_{u \in \left\{ \frac{1}{M}, \dots, 1 \right\}^N} \prod_{i=1}^N f_i(u_i) \ln \left( \frac{\prod_{i=1}^N f_i(u_i)}{g(u)} \right) \\ &= \operatorname{argmin}_{f_1, \dots, f_N} \sum_{u \in \left\{ \frac{1}{M}, \dots, 1 \right\}^N} \prod_{i=1}^N f_i(u_i) \ln \left( \prod_{i=1}^N f_i(u_i) \right) \\ &\quad + N \ln(M), \end{aligned} \tag{3.5.15}$$

Subject to:

$$\begin{aligned} \sum_{u_i} f_i(u_i) &= 1, i = 1, \dots, N \\ \sum_{u_i} \sum_{u_i > u_j} f_i(u_i) f_j(u_j) &= \alpha_{ij}, i, j = 1, \dots, N, i \neq j, \end{aligned} \tag{3.5.16}$$

with

$$0 \leq f_1(u_1), \dots, f_N(u_N) \leq 1$$

$$u_i = \left\{ \frac{1}{M}, \dots, 1 \right\}, i = 1 \dots N$$

The gradients of  $f_1(u_1), \dots, f_N(u_N)$  given the Lagrangian are :

$$\begin{aligned}
\frac{\partial L}{\partial f_1(u_1)} &= \sum_{u_2, \dots, u_N = \frac{1}{M}}^1 f_2(u_2) \dots f_N(u_N) [\ln(f_1(u_1) \dots f_N(u_N)) + 1] + \lambda_1 \\
&+ \lambda_{12} \sum_{u_2 = u_1 + \frac{1}{N}}^1 f_2(u_2) + \dots + \lambda_{1N} \sum_{u_N = u_1 + \frac{1}{M}}^1 f_N(u_N) \\
\frac{\partial L}{\partial f_2(u_2)} &= \sum_{u_1, u_3, \dots, u_N = \frac{1}{M}}^1 f_1(u_1) f_3(u_3) \dots f_N(u_N) [\ln(f_1(u_1) \dots f_N(u_N)) + 1] + \lambda_2 \\
&+ \lambda_{21} \sum_{u_1 = \frac{1}{M}}^{u_2 - \frac{1}{M}} f_1(u_1) + \dots + \lambda_{2N} \sum_{u_N = u_2 + \frac{1}{M}}^1 f_N(u_N) \\
&\dots = \dots \\
&\dots = \dots \\
&\dots = \dots \\
\frac{\partial L}{\partial f_N(u_N)} &= \sum_{u_1, \dots, u_{N-1} = \frac{1}{M}}^1 f_1(u_1) \dots f_{N-1}(u_{N-1}) [\ln(f_1(u_1) \dots f_N(u_N)) + 1] + \lambda_N \\
&+ \lambda_{N1} \sum_{u_1 = \frac{1}{M}}^{u_N - \frac{1}{M}} f_1(u_1) + \dots + \lambda_{NN-1} \sum_{u_{N-1} = \frac{1}{M}}^{u_N - \frac{1}{M}} f_{N-1}(u_{N-1}). \tag{3.5.17}
\end{aligned}$$

Putting the gradients equal to zero gives a system of non-linear equations

$$\begin{aligned}
 \ln(f_1) &= - \sum_{u_2, \dots, u_N} f_2(u_2) \dots f_N(u_N) \ln(f_2(u_2) \dots f_N(u_N)) - 1 - \lambda_1 \\
 &\quad - \lambda_{12} \sum_{u_2=u_1+\frac{1}{M}}^1 f_2(u_2) - \dots - \lambda_{1N} \sum_{u_N=u_1+\frac{1}{M}}^1 f_N(u_N) \\
 \ln(f_2) &= - \sum_{u_1, u_3, \dots, u_N} f_1(u_1) f_3(u_3) \dots f_N(u_N) \ln(f_1(u_1) \dots f_N(u_N)) \\
 &\quad - 1 - \lambda_2 - \lambda_{21} \sum_{u_1=\frac{1}{M}}^{u_2-\frac{1}{M}} f_1(u_1) - \dots - \lambda_{2N} \sum_{u_N=u_2+\frac{1}{M}}^1 f_N(u_N) \\
 &\quad \dots = \dots \\
 &\quad \dots = \dots \\
 &\quad \dots = \dots \\
 \ln(f_N) &= - \sum_{u_1, \dots, u_{N-1}} f_1(u_1) \dots f_{N-1}(u_{N-1}) \ln(f_1(u_1) \dots f_{N-1}(u_{N-1})) \\
 &\quad - 1 - \lambda_N - \lambda_{N1} \sum_{u_1=\frac{1}{M}}^{u_N-\frac{1}{M}} f_1(u_1) - \dots \\
 &\quad - \lambda_{NN-1} \sum_{u_{N-1}=\frac{1}{M}}^{u_N-\frac{1}{M}} f_{N-1}(u_{N-1}). \tag{3.5.18}
 \end{aligned}$$

which can be written as a system of recurrence relations.

$$\begin{aligned}
 f_1\left(u_1 + \frac{1}{M}\right) &= f_1(u_1) e^{\sum_{j=2}^N \lambda_{1j} f_j(u_j + \frac{1}{M})} \\
 f_2\left(u_2 + \frac{1}{M}\right) &= f_2(u_2) e^{-\lambda_{12} f_1(u_1) + \sum_{j=3}^N \lambda_{2j} f_j(u_j + \frac{1}{M})} \\
 &\quad \dots = \dots \\
 &\quad \dots = \dots \\
 &\quad \dots = \dots \\
 f_N\left(u_N + \frac{1}{M}\right) &= f_N(u_N) e^{-\sum_{j=1}^{N-1} \lambda_{Nj} f_j(u_j + \frac{1}{M})}. \tag{3.5.19}
 \end{aligned}$$

As with the case of two choice alternatives the problem is to find  $f_1\left(\frac{1}{M}\right), f_2\left(\frac{1}{M}\right), \dots, f_N\left(\frac{1}{M}\right)$  and  $\lambda_{12}, \lambda_{13}, \dots, \lambda_{N(N-1)}$  such that the constraints are met with  $\lambda_{ij} = \lambda_{ji}$ .

## Derivation Minimal Informative Distribution over Two Choice Alternatives and with Independent Normal Marginals

The problem of finding a minimally informative distribution relative to a standard normal distribution and paired comparison data

$$\operatorname{argmin}_{\bar{\mu}, \Sigma} I(f|g) = \operatorname{argmin}_{\bar{\mu}, \Sigma} \frac{1}{2} (\mu_1^2 + \mu_2^2) + \frac{1}{2} (\sigma_1^2 + \sigma_2^2) - \frac{1}{2} \ln (\sigma_1^2 \sigma_2^2 - \rho^2 \sigma_1^2 \sigma_2^2) - 1, \quad (3.5.20)$$

Subject to:

$$\frac{\mu_1 - \mu_2}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2}} = \Phi^{-1}(\alpha) \quad (3.5.21)$$

The Lagrangian is

$$\begin{aligned} \mathcal{L}(\bar{\mu}, \bar{\sigma}, \rho, \lambda) &= \frac{1}{2} (\mu_1^2 + \mu_2^2) + \frac{1}{2} (\sigma_1^2 + \sigma_2^2) \\ &\quad - \frac{1}{2} \ln (\sigma_1^2 \sigma_2^2) - \frac{1}{2} \ln (1 - \rho^2) - 1 \\ &\quad + \lambda \left( \frac{\mu_1 - \mu_2}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2}} - \delta \right). \end{aligned} \quad (3.5.22)$$

Deriving the derivatives of the Lagrangian with respect to  $\bar{\mu}, \bar{\sigma}, \rho, \lambda$  and setting them to zero gives

$$\frac{\partial L}{\partial \mu_1} = \mu_1 + \frac{\lambda}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2}} = 0 \quad (3.5.23)$$

$$\frac{\partial L}{\partial \mu_2} = \mu_2 - \frac{\lambda}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2}} = 0 \quad (3.5.24)$$

$$\frac{\partial L}{\partial \sigma_1} = \sigma_1 - \frac{1}{\sigma_1} - \frac{\lambda (\mu_1 - \mu_2) (\sigma_1 - \rho^2 \sigma_2)}{(\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2)^{\frac{3}{2}}} = 0 \quad (3.5.25)$$

$$\frac{\partial L}{\partial \sigma_2} = \sigma_2 - \frac{1}{\sigma_2} - \frac{\lambda (\mu_1 - \mu_2) (\sigma_2 - \rho^2 \sigma_1)}{(\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2)^{\frac{3}{2}}} = 0 \quad (3.5.26)$$

$$\frac{\partial L}{\partial \rho} = \frac{\rho}{1 - \rho^2} + \frac{2\lambda (\mu_1 - \mu_2) \rho \sigma_1 \sigma_2}{(\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2)^{\frac{3}{2}}} = 0 \quad (3.5.27)$$

$$\frac{\partial L}{\partial \lambda} = \frac{\mu_1 - \mu_2}{\sqrt{\sigma_1^2 + \sigma_2^2 - 2\rho^2 \sigma_1 \sigma_2}} - \delta = 0. \quad (3.5.28)$$

Adding (3.5.23) and (3.5.24) gives.

$$\mu_1 + \mu_2 = 0 \quad (3.5.29)$$

For convenience we set

$$a = \frac{\lambda(\mu_1 - \mu_2)}{(\sigma_1^2 + \sigma_2^2 - 2\rho^2\sigma_1\sigma_2)^{\frac{3}{2}}}. \quad (3.5.30)$$

Multiplying (3.5.25) and (3.5.26) respectively with  $\sigma_1$  and  $\sigma_2$  gives.

$$\sigma_1(1-a) = 1 - a\rho^2\sigma_1\sigma_2 \quad (3.5.31)$$

$$\sigma_2(1-a) = 1 - a\rho^2\sigma_1\sigma_2. \quad (3.5.32)$$

From (3.5.31) and (3.5.32) it follows that

$$\sigma_1 = \sigma_2. \quad (3.5.33)$$

From (3.5.27) and (3.5.33) it follows that

$$\rho \left( \frac{1}{1-\rho^2} + 2a\sigma_1^2 \right) = 0, \quad (3.5.34)$$

which gives

$$\rho = 0 \vee \frac{1}{1-\rho^2} + 2a\sigma_1^2 = 0. \quad (3.5.35)$$

For  $\rho = 0$  the term  $-\frac{1}{2} \ln(1-\rho^2)$  is minimal. Substituting  $\mu_2 = -\mu_1$ ,  $\sigma_2 = \sigma_1$  and  $\rho = 0$  into (3.5.28) gives

$$\mu_1 = \frac{1}{2} \sqrt{2} \sigma_1 \delta. \quad (3.5.36)$$

Substituting (3.5.36) into (3.5.23) gives

$$\lambda = -\sigma_1^2 \delta. \quad (3.5.37)$$

Substituting (3.5.37) into (3.5.25) gives

$$\sigma_1 = \sqrt{\frac{2}{2+\delta^2}} \vee \sigma_1 = -\sqrt{\frac{2}{2+\delta^2}}. \quad (3.5.38)$$

But the standard deviation has to be bigger than zero. After substituting the result of (3.5.38) into the other equation it follows that

$$\mu_1^* = \delta \sqrt{\frac{1}{2+\delta^2}}, \mu_2^* = -\delta \sqrt{\frac{1}{2+\delta^2}}$$

$$\sigma_1^* = \sqrt{\frac{2}{2 + \delta^2}}, \sigma_2^* = \sqrt{\frac{2}{2 + \delta^2}}, \rho^* = 0$$

$$\delta = \Phi^{-1}(\alpha)$$





# Application to Prioritizing Marine Ecosystem Vulnerabilities<sup>1</sup>

## 4.1 Background

This study presents an analysis of 64 experts' rankings of 30 scenarios of human activities and their impacts to coastal ecosystems. The elicitation protocols were designed and executed by researchers at the National Center for Ecological Analysis and Synthesis. Experts were asked to rank the five scenarios posing the greatest threats and the five scenarios posing the least threats. The goal of this study was to find weights for criteria that adequately model these stakeholders' preferences and can be used to predict the scores of other scenarios. Probabilistic inversion (PI) techniques were used to quantify a model of ecosystem vulnerability based on five criteria. Stakeholder preference modeling can also serve as a form of expert elicitation when the stakeholders are domain experts, as in the present case. Their preferences are taken to prioritize threats to marine ecosystems, with a view to optimizing mitigation and abatement actions.

Other multicriteria weighting methods [51, 27, 52] require stakeholders to evaluate the criteria directly. However, the weights assigned to a criterion cannot be assessed independently of the scale on which all criteria scores are measured this is a fact that is sometimes overlooked. The present approach asks the stakeholders to rank scenarios rather than evaluate criteria. Criteria weights are then derived to fit the stakeholder preference rankings as well as possible. This has the significant advantage of allowing us to assess the validity of our fitted model of stakeholder preference.

Probabilistic inversion denotes the operation of inverting a function over a pro-

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<sup>1</sup>This chapter is based on Neslo et al. [71]

bability distribution, rather than at a point. Such problems arise in quantifying uncertainty in physical models [17, 42, 43, 41, 56]. One has uncertainty distributions on observable phenomena, either from data or from expert judgment, and one wishes to find a distribution over the parameters of a predictive model, such that one recovers the observed distributions when the parameter distributions are *pushed through* the model. PI algorithms used in the past were computationally intensive, involving sophisticated interior point optimization techniques and duality theory as well as ad hoc steering [39]. Recent computational advances [58, 98] clarify the mathematical foundations for PI and yield simple algorithms with proven convergence behavior, suitable for use by nonspecialists. The results depend on a variant of the classical Iterative Proportional Fitting algorithm [13, 16, 17, 34, 44, 46, 47, 58].

In stakeholder preference modeling, the data is discrete-choice preference data elicited from a set of stakeholders. The distributions to be inverted are those of indicator variables, for example:

- Alternative  $i$  is better than alternative  $j$ .
- Alternative  $i$  is ranked third in the given set of alternatives.

We are interested in the probability of such variables, taking the values "yes" or "no" for a set of stakeholders. We can measure these probabilities by querying a large representative set of stakeholders. Existing discrete-choice or random-utility techniques construct a value or utility function from discrete-choice data [2, 5, 56, 55, 60, 85, 91, 94, 96, 95], and they strongly restrict the form of the utility functions. Using PI, this form can be inferred from choice data.

We first discuss the model, then address model adequacy and model fit. Summary statistics for the 30 scenarios are then given. The conclusion of this analysis is that the data are broadly consistent with a linear model of stakeholder preferences.

## 4.2 The Model

In this study there were 64 experts ranking 30 threat scenarios based on the scores of five criteria:

These criteria were developed and tested elsewhere [31, 11, 66, 88]. The score (utility) of threat scenario  $i$  for stakeholder  $s$  is modeled as:

$$u_s(a_i) = \sum_{j=1}^5 \omega_{s,j} \times c_{i,j}; \sum_{j=1}^5 \omega_{s,j} = 1; \omega_{s,j} > 0. \quad (4.2.1)$$

The weights are non-negative random variables that sum to 1. The (joint) distribution for the weights is modeled to represent the distribution of weights in a population of stakeholders, of which the 64 elicited experts are a random

**Table 4.2.1:** *Threat criteria definition*

Name	Description	Unit	Range
$C_1$	Spatial scale	$km^2$	0.1-50000
$C_2$	Frequency	$\#/yr$	1-360
$C_3$	Trophic (functional) impact	—	1-4
$C_4$	Recovery time	$yr s$	1-50
$C_5$	Resistance	%	5-75

sample. Since the weights are normalized, the criteria are transformed so that the product  $\omega_{s,j} \times c_{i,j}$  is positive and falls roughly within the same range. Spatial scale is given in square kilometers, and the values for spatial scale range from 0.1 to 50,000  $km^2$ . These values are transformed to  $\ln(100 * m^2)$ , whose values thus range from 2.3 to 15.4. Frequency was scored as  $\ln(360 * /year)$ . Trophic or functional impact is the number of trophic layers affected. Resistance is scored as the percent of species affected per trophic layer. These transformations are chosen for mathematical convenience.

A salient feature of these data is dominance. Scenario  $a_i$  dominates Scenario  $a_j$  from above if  $a_i$ 's scores on all five criteria are greater or equal to the scores of  $a_j$ .  $a_i$  dominates  $a_j$  from below if  $a_i$ 's scores on all five criteria are less than or equal to those of  $a_j$ . If  $a_i$  dominates  $a_j$  from above, then  $a_j$  can never be ranked above  $a_i$  in any model that computes the scenario score as a monotonic function of the five criteria scores. The presence of dominated scenarios enables us to analyze whether the experts' rankings are broadly consistent with a monotonic model of criteria scores.

## 4.3 Results and Validation

### 4.3.1 Model Adequacy

Of the 30 scenarios, only seven were non-dominated. This means that none of the 23 scenarios dominated from above could be ranked 1 by a stakeholder whose preferences were consistent with the model. In fact, 22.4% of the top rankings were inconsistent in this sense: 77.6% of the top rankings went to four of the seven non-dominated scenarios. A scenario dominated from above by two or more scenarios could not consistently be ranked second; in fact, 23.7% of the second rankings were inconsistent in this sense. Dominance from below was much less prevalent than dominance from above.

In view of the large number of dominated scenarios, we view the percentages of inconsistent rankings as indicating that the stakeholders' preferences were broadly, though not wholly, consistent with a monotonic model<sup>2</sup>. We therefore

<sup>2</sup>If the 64 experts had chosen their top-ranked scenario at random, the probability that 14 or fewer

proceeded to fit the linear model (4.2.1).

The 30 scenarios and their criteria scores are shown in Table 4.3.1. The non-dominated scenarios are shaded.

**Table 4.3.1:** Scenario and Criteria Scores

Nr	Code	Scenario	Scale	Freq	Func	Recov	Resist
1	am	Aquaculture: marine plant	5.30	11.77	1	1	0.2
2	as	Aquaculture: shellfish	6.21	11.77	1	0.1	0.05
3	cl	Climate change: sea level rise	13.82	5.19	2	5	0.2
4	ct	Climate change: sea temp	15.42	5.89	3	50	0.25
5	cu	Climate change: UV	13.82	3.58	1	1	0.05
6	ca	Coastal engineering: habitat alteration	4.61	5.89	4	25	0.75
7	dh	Direct human impact: trampling	9.62	11.77	2	25	0.35
8	fd	Fishing: demersal destructive	6.68	2.89	4	0.5	0.1
9	fn	Fishing: demersal non-destructive low bycatch	2.30	2.89	1	0.5	0.1
10	fa	Fishing: non-destructive artisanal	4.61	2.89	1	1	0.5
11	fp	Fishing: pelagic high bycatch	6.21	1.28	1	0.5	0.05
12	fr	Fishing: recreational	6.68	9.84	2	5	0.2
13	fu	Freshwater input: increase	6.91	4.28	2	1	0.1
14	is	Invasive species	14.51	11.77	1	20	0.25
15	ma	Military activity	6.91	8.37	1	5	0.1
16	nh	Nutrient input: causing HAMS	9.21	4.28	2	1	0.1
17	nz	Nutrient input: causing hypoxic zones	6.68	4.28	3	1	0.05
18	no	Nutrient input: into oligotrophic waters	8.29	4.97	1	0.5	0.3
19	og	Ocean dumping: lost fishing gear	2.30	5.89	3	3	0.15
20	os	Ocean dumping: ship wrecks	3.91	2.89	4	10	0.5
21	ox	Ocean dumping: toxic materials	6.91	2.89	1	1	0.1
22	po	Ocean pollution	6.91	6.58	1	3	0.2
23	pa	Pollution input: atmospheric	9.62	3.58	1	0.5	0.2
24	pi	Pollution input: inorganic	8.29	4.28	2	3	0.2
25	pr	Pollution input: organic	8.52	5.19	2	5	0.2
26	ps	Power, desalination plants	4.61	11.77	3	10	0.5
27	sr	Scientific research: collecting	2.30	8.37	1	2	0.15
28	sd	Sediment input: decrease	3.91	1.28	1	0.5	0.05
29	si	Sediment input: increase	10.82	5.19	2	10	0.3
30	ts	Tourism: surfing	2.30	10.49	1	1	0.05

would chose one of the 23 dominated scenarios is in the order of  $10^{20}$ .

### 4.3.2 Criteria Weights

We fit the linear model by finding a distribution over criteria weights which fit as well as possible the probabilities of rankings given by the stakeholders. The fitting is done by probabilistic inversion. We start with a non-informative distribution over criteria weights (which however are constrained to add to 1). We then adapt this distribution to optimally recover the stakeholders' rankings. That is, if we sample randomly from the adapted distribution, the probability of drawing a set of weights with which Scenario  $a_i$  is ranked first equals, to the extent possible, the percentage of experts who ranked  $a_i$  first, and so on. The fitting based on first ranks applies only to the percentages for the scenarios that were ranked first. Similarly, the fitting based on the first two ranks applies only to the percentages for the scenarios ranked 1 or 2.

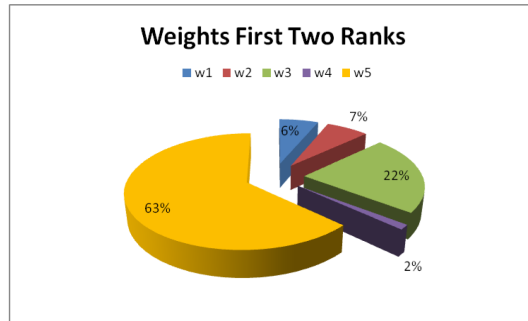
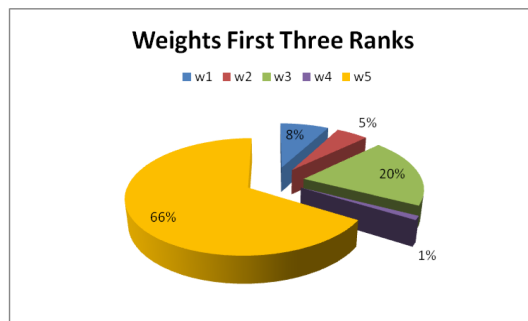
We are interested in finding a fitting that can be validated by predicting rankings *not* used in the fitting, also known as out-of-sample validation. Since the goal is to prioritize threats, the top rankings are most important. Satisfactory results were found by fitting the model based on the first four rankings; this model could then be used to predict the fifth rankings. Table 4.3.2 and Figure 4.3.14 compare the predicted and observed percentages of rankings. The model is first used to "retrodict" or "recover" the first four rankings. These are the data actually used to fit the model, so this comparison is a check of model fit rather than model prediction. Using the model, we can predict the percentages of experts ranking the various scenarios in the fifth position (Figure 4.3.14). These percentages were not used in fitting the model and test the ability of the model to predict preferences of the population of stakeholders. Of course, we should hope that the predictions and retrodictions show similar agreement with the observed rankings.

Because we are fitting a linear model, the expected score of any scenario may be computed by using the expected values of the criteria weights in the adapted distribution. A new scenario, not among the original 30, can be scored by multiplying its (transformed) criteria scores by the expected weight of each criterion. This of course is the great advantage of a linear model, and explains the preference for this model above more complex models, even though the latter might yield a better fit. Figures 4.3.1 to 4.3.5 show the expected criteria weights based on fitting only the first ranks, the first two ranks, the first three ranks, and the first four ranks, and finally, based on fitting all ranks.

We observe that these expected weights do not change significantly between the two-, three-, and four-rank options. Using all ranks causes changes, and also causes greater variance in the criteria scores (see Table 4.3.4).

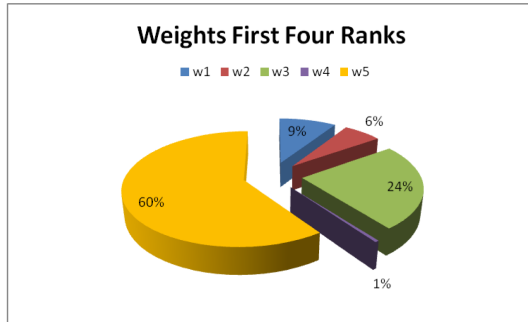
Although the expected weights are most important in using the model, it is also of interest to examine the distributions of weights. Figures 4.3.6 to 4.3.10 shows the cumulative distribution functions of the five weights in the four cases shown in Figures 4.3.1 to 4.3.5.

The joint distributions for rank one, ranks one and two, ranks one to three, ranks one to four, and all ranks are shown in Figures 4.3.11 to 4.3.13.

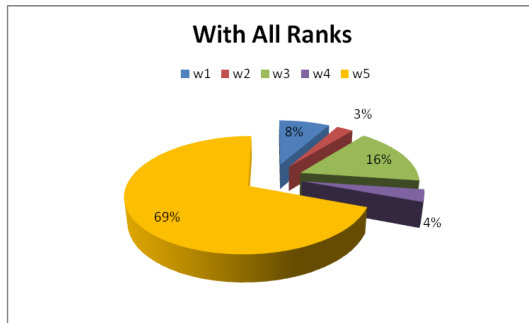
**Figure 4.3.1:** *Expected criteria weights based on ranks 1***Figure 4.3.2:** *Expected criteria weights based on ranks 1,2***Figure 4.3.3:** *Expected criteria weights based on ranks 1,2,3*

The rightmost cumulative distributions indicate greatest importance. The pictures from Figures 4.3.6 to 4.3.10 echoes that in Figures 4.3.1 to 4.3.5 for the first two ranks: resistance is most important, followed by trophic impact. Of course, we must bear in mind that these results are relative to the scaling chosen

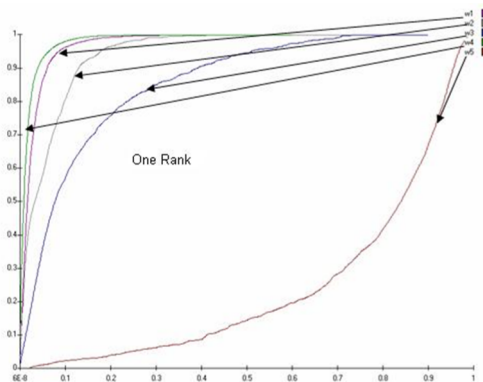
**Figure 4.3.4:** *Expected criteria weights based on ranks 1,2,3,4*



**Figure 4.3.5:** *Expected criteria weights based on all ranks*

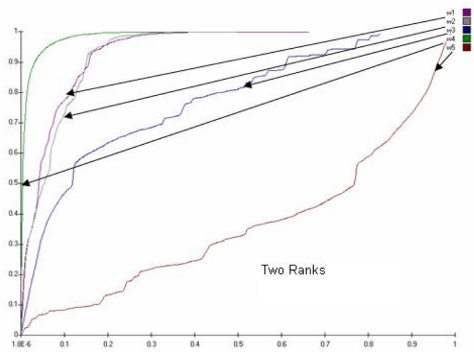
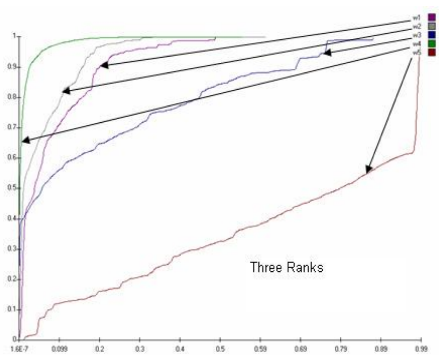
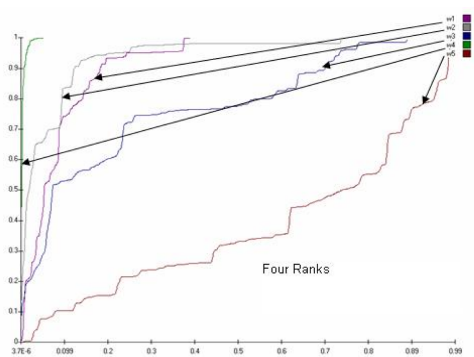


**Figure 4.3.6:** *Cumulative weight distributions based on ranks 1*



to represent the criteria scores.

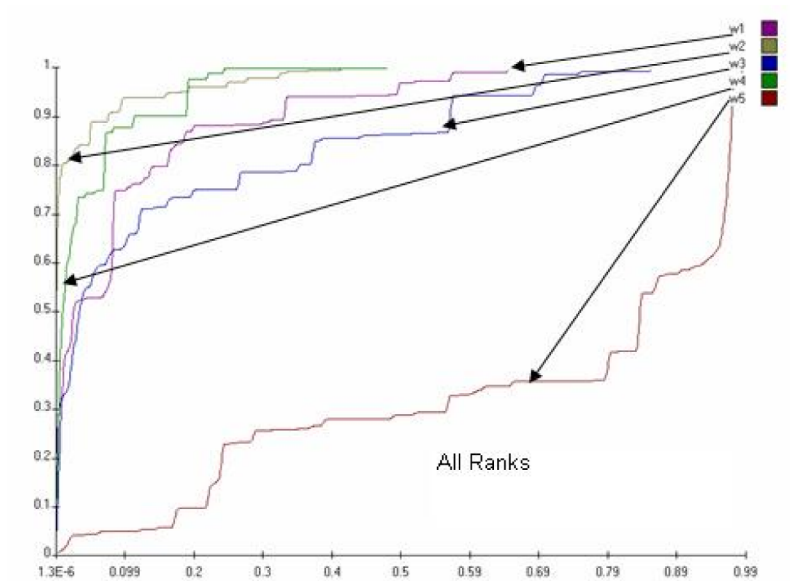
Figures 4.3.1 to 4.3.5 and 4.3.6 to 4.3.10 show that the mean values and

**Figure 4.3.7:** *Cumulative weight distributions based on ranks 1,2***Figure 4.3.8:** *Cumulative weight distributions based on ranks 1,2,3***Figure 4.3.9:** *Cumulative weight distributions based on ranks 1,2,3,4*

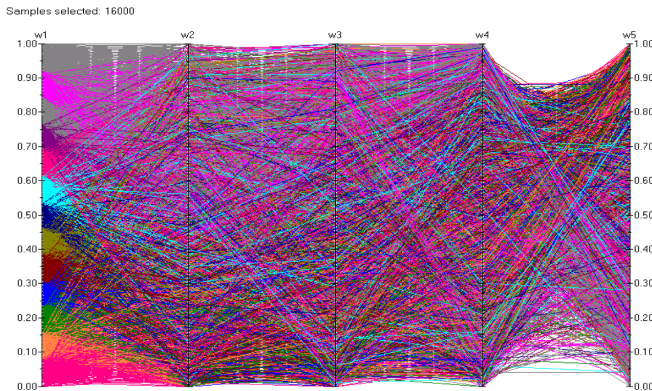
marginal distributions are somewhat similar in all fitting situations. The joint dis-



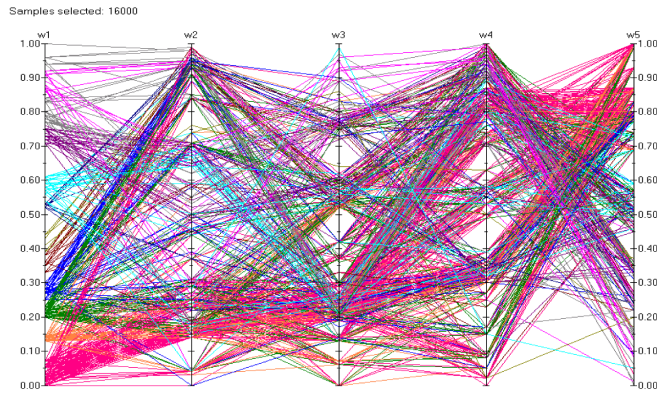
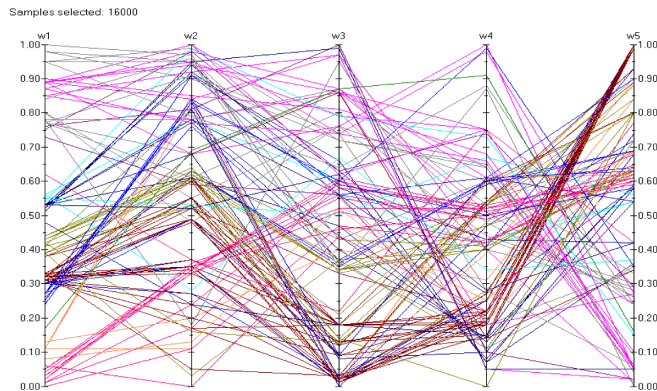
**Figure 4.3.10:** Cumulative weight distributions based on all ranks



**Figure 4.3.11:** Percentile cobweb plots for criteria weights based on fitting ranks 1



tributions, however, are quite different. One sample of weights represents one virtual stakeholder. If we plot these five weights on five vertical lines, we get a jagged line representing one virtual stakeholder. If we plot 16,000 such lines we get a picture of the population of stakeholders. We say that the stakeholder weights have interactions if, for example, knowledge that a stakeholder assigns

**Figure 4.3.12:** *Percentile cobweb plots for criteria weights based on fitting ranks 1,2,3,4***Figure 4.3.13:** *Percentile cobweb plots for criteria weights based on fitting ranks all ranks*

high weight to the "frequency" criterion gives significant information regarding weights for other criteria. A quick visual impression of the joint distributions is given by the "percentile cobweb plots" shown in Figure 3. Instead of the weights themselves, Figures 4.3.11 to 4.3.13 plot the weights' percentiles, as this makes the dependence structure more visible. Evidently the joint distributions are complex, and are different for the different fitting situations. A detailed analysis of interactions is not undertaken here. It is worth noting that the probabilistic inversion infers the dependence structure from the stakeholder data; it does not assume or impose any structure. We note that as we use more ranks in the fitting, the fitting becomes less smooth. The departure from the starting distribution grows more pronounced as the number of constraints that the fitting tries to satisfy increases.

Table 4.3.2 shows the predicted probabilities of rankings based on the fitting in the four cases discussed above. Thus "prediction I" indicates the prediction based on fitting only the first-ranked scenarios. The first column gives the constraints. "#S4=1" denotes the constraint that Scenario 4 was ranked 1. The last column shows that 34.33% of the stakeholders ranked Scenario 4 as 1. Using the fitting based only on the first ranks predicts that 34.24% of the population of stakeholders would rank Scenario 4 as 1. Similarly, using the fitting based on the first four ranks, 43.59% of the population would rank Scenario 4 first. Of course, owing to the presence of inconsistent rankings, the fitting can never be perfect. Indeed, 22.4% of the first ranks were inconsistent with the model; as we fit 77.6% of the consistent rankings, the remaining probability mass must be distributed over the other feasible rankings. Some of the discrepancies are sizeable, as in the case of #S20 = 5 for the prediction based in the top four ranks. On the whole, however, the predictions do capture the drift of stakeholder preferences. Fitting all ranks is numerically quite burdensome and conflates issues that determine the most serious and least serious threats. The fitting based on the top four rankings presents the best compromise.

**Table 4.3.2:** Model predictions and stakeholder probabilities for top 5 rankings

Constraint	Prediction I	Prediction I,II	Prediction I,II,III	Prediction I,II,III,IV	Stakeholders
#S3=1	0.0000	0.0000	0.0000	0.0000	0.0597
#S4=1	0.3424	0.3428	0.3420	0.4359	0.3433
#S6=1	0.2695	0.2687	0.4164	0.3008	0.2687
#S7=1	0.0296	0.0299	0.0453	0.0329	0.0299
#S8=1	0.0000	0.0000	0.0114	0.0000	0.0149
#S9=1	0.0000	0.0000	0.0000	0.0000	0.0149
#S11=1	0.0000	0.0000	0.0000	0.0000	0.0149
#S12=1	0.0000	0.0000	0.0000	0.0000	0.0149
#S14=1	0.0744	0.0748	0.0580	0.0800	0.0746
#S16=1	0.0000	0.0000	0.0000	0.0000	0.0299
#S19=1	0.0000	0.0000	0.0000	0.0000	0.0149
#S22=1	0.0000	0.0000	0.0000	0.0000	0.0448
#S25=1	0.0000	0.0000	0.0000	0.0000	0.0149
#S28=1	0.0000	0.0000	0.0000	0.0000	0.0299
#S29=1	0.0000	0.0000	0.0000	0.0000	0.0299
#S2=2	0.0000	0.0000	0.0000	0.0000	0.0339
#S3=2	0.0001	0.0339	0.0442	0.0392	0.0339
#S4=2	0.2295	0.2213	0.1713	0.2218	0.2203
#S5=2	0.0000	0.0000	0.0000	0.0000	0.0169
#S6=2	0.4753	0.0511	0.0663	0.0661	0.0508
#S7=2	0.1557	0.0676	0.0825	0.0681	0.0678
#S8=2	0.0000	0.0679	0.0432	0.0725	0.0678
#S9=2	0.0000	0.0000	0.0000	0.0000	0.0169
#S11=2	0.0000	0.0000	0.0000	0.0000	0.0169
#S14=2	0.0275	0.2700	0.1855	0.2829	0.2712
#S16=2	0.0000	0.0000	0.0000	0.0000	0.0508
#S18=2	0.0000	0.0000	0.0000	0.0000	0.0169
#S20=2	0.0238	0.0170	0.0214	0.0174	0.0169
#S22=2	0.0000	0.0000	0.0000	0.0000	0.0508
#S23=2	0.0000	0.0000	0.0000	0.0000	0.0169
#S24=2	0.0000	0.0000	0.0000	0.0000	0.0169

Table 4.3.2 – continued from previous page

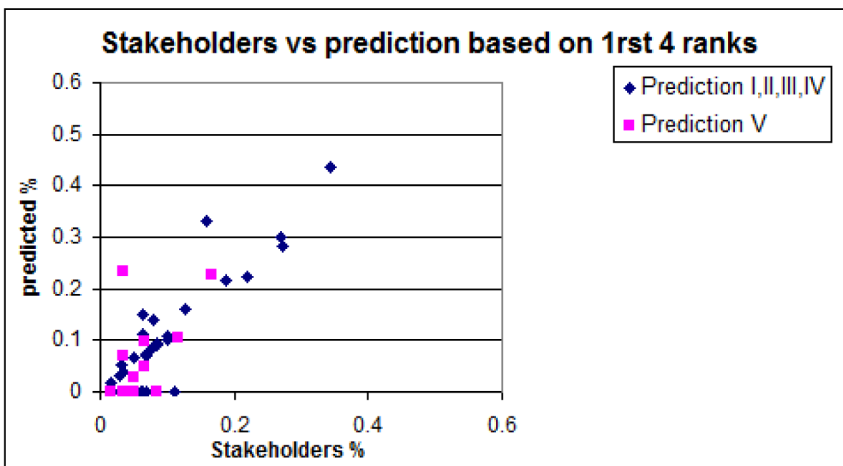
Constraint	Prediction I	Prediction I,II	Prediction I,II,III	Prediction I,II,III,IV	Stakeholders
#S29=2	0.0000	0.0000	0.0000	0.0000	0.0508
#S2=3	0.0000	0.0000	0.0000	0.0000	0.0317
#S3=3	0.0015	0.0084	0.1924	0.3305	0.1587
#S4=3	0.0798	0.0656	0.0769	0.1486	0.0635
#S6=3	0.0707	0.2063	0.0713	0.1131	0.0635
#S7=3	0.5732	0.4615	0.0816	0.1401	0.0794
#S8=3	0.0005	0.0053	0.0328	0.0514	0.0317
#S9=3	0.0000	0.0000	0.0000	0.0000	0.0159
#S12=3	0.0000	0.0000	0.0000	0.0000	0.0635
#S14=3	0.0730	0.0649	0.1276	0.1616	0.1270
#S16=3	0.0000	0.0000	0.0000	0.0000	0.0317
#S17=3	0.0000	0.0000	0.0000	0.0000	0.0635
#S18=3	0.0000	0.0000	0.0000	0.0000	0.0317
#S20=3	0.0968	0.1582	0.0158	0.0189	0.0159
#S21=3	0.0000	0.0000	0.0000	0.0000	0.0159
#S22=3	0.0000	0.0000	0.0000	0.0000	0.0159
#S24=3	0.0000	0.0000	0.0000	0.0000	0.0159
#S25=3	0.0000	0.0000	0.0000	0.0000	0.1111
#S26=3	0.1044	0.0293	0.0160	0.0181	0.0159
#S29=3	0.0000	0.0000	0.0000	0.0000	0.0794
#S3=4	0.0137	0.0687	0.0137	0.2174	0.1864
#S4=4	0.1508	0.1125	0.0150	0.0392	0.0339
#S5=4	0.0001	0.0036	0.0372	0.0392	0.0339
#S6=4	0.0889	0.3417	0.2099	0.0958	0.0847
#S7=4	0.1196	0.1948	0.2580	0.1091	0.1017
#S8=4	0.0031	0.0074	0.0028	0.0737	0.0678
#S11=4	0.0000	0.0000	0.0000	0.0000	0.0339
#S12=4	0.0017	0.0000	0.0000	0.0000	0.0847
#S14=4	0.2851	0.0784	0.0235	0.0910	0.0847
#S16=4	0.0000	0.0000	0.0000	0.0000	0.0339
#S17=4	0.0000	0.0000	0.0000	0.0000	0.0169
#S18=4	0.0000	0.0000	0.0000	0.0000	0.0169
#S20=4	0.0990	0.0795	0.3630	0.0176	0.0169
#S22=4	0.0000	0.0000	0.0000	0.0000	0.0678
#S24=4	0.0000	0.0000	0.0000	0.0000	0.0169
#S25=4	0.0000	0.0000	0.0000	0.0000	0.0508
#S29=4	0.0000	0.0001	0.0000	0.1024	0.1017
#S2=5	0.0122	0.0024	0.0035	0.0705	0.0333
#S3=5	0.0140	0.0845	0.0276	0.0000	0.0500
#S4=5	0.1189	0.1671	0.0182	0.0270	0.0500
#S6=5	0.0544	0.0789	0.0974	0.0969	0.0667
#S7=5	0.1121	0.1460	0.4151	0.2279	0.1667
#S8=5	0.0034	0.0091	0.0057	0.0000	0.0167
#S12=5	0.0094	0.0005	0.0000	0.0004	0.0167
#S13=5	0.0000	0.0000	0.0000	0.0000	0.0167
#S14=5	0.1848	0.1641	0.1137	0.1036	0.1167
#S16=5	0.0000	0.0000	0.0000	0.0000	0.0833
#S17=5	0.0000	0.0000	0.0114	0.0000	0.0167
#S19=5	0.0000	0.0000	0.0000	0.0000	0.0167
#S20=5	0.1714	0.0864	0.0883	0.2331	0.0333
#S22=5	0.0000	0.0000	0.0000	0.0000	0.0333
#S24=5	0.0000	0.0000	0.0000	0.0000	0.0167

Table 4.3.2 – continued from previous page

Constraint	Prediction I	Prediction I,II	Prediction I,II,III	Prediction I,II,III,IV	Stakeholders
#S25=5	0.0000	0.0000	0.0000	0.0000	0.0500
#S26=5	0.2552	0.1646	0.1003	0.0493	0.0667

Figure 4.3.14 shows the information in Table 4.3.2 graphically. On the horizontal axis are stakeholders' percentages for rankings of scenarios; on the vertical axis are the predicted percentages based on the fitted model. The diamonds are scenarios which were ranked first, second, third, or fourth. These percentages were used to fit the model. The squares are scenarios that were ranked fifth. We see that these percentages are reasonably well predicted by the model. Scenarios plotted on the horizontal axis correspond to rankings that are inconsistent with the model.

Figure 4.3.14: Predictions based on ranks 1 to 4, of stakeholder percentages for first four ranks (diamonds), and for 5th ranks (squares)



### 4.3.3 Scenario Scores

Figure 4.3.15 shows the densities of the scores of the top four scenarios, ranked according to their mean values. These densities are generated by the distribution of criteria weights, which models the distribution of participants. It is interesting to note that the modes of these densities are all similar, but the shapes are different. The top-ranked scenario, Scenario 4 (Sea level rise), is distinguished by a large right tail. Scenario 6 (Coastal engineering) shows a bimodal form, suggesting that there are two distinct subgroups of participants. The remaining two

scenarios, Scenario 14 (Invasive species) and Scenario 7 (Direct human impact) are quite similar in distribution.

**Figure 4.3.15:** *Densities for the top 4 ranked scenarios*

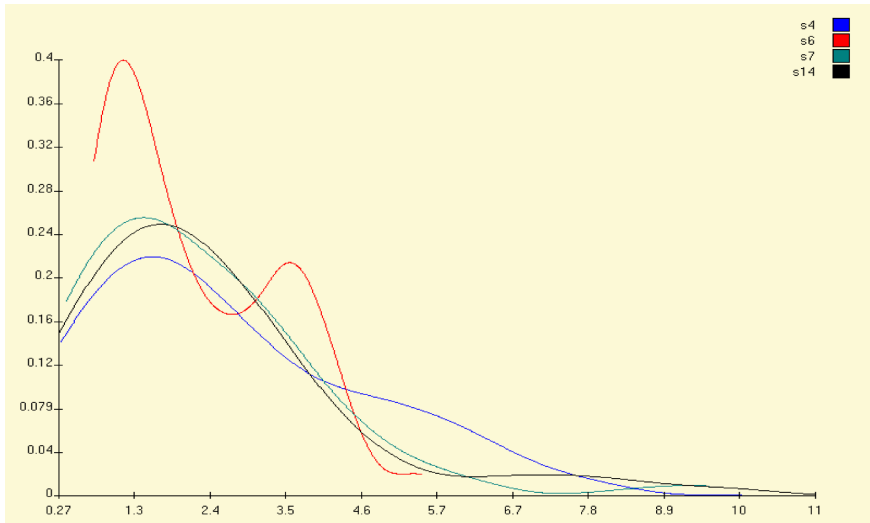


Table 4.3.3 shows the mean, variance, and standard deviation of the five criteria weights and the 30 scenarios, based on the first four ranks. Table 4.3.4 gives the same information based on all ranks. Note that the variances in Table 4.3.4 tend to be larger, sometimes much larger. The top-ranked Scenario 4 has a variance of 3.7 based on four ranks, and 17.2 based on all ranks. This suggests that trying to fit the top and bottom ranks just makes the problem more infeasible—it does not give more insight into the factors determining high-threat scenarios.

**Table 4.3.3:** *With First four Rank*

Variable	Mean	Variance	SD
S1	1.572	1.362	1.167
S2	1.561	1.523	1.234
S3	2.214	2.103	1.450
S4	2.901	3.702	1.924
S5	1.763	1.649	1.284
S6	2.328	1.464	1.210
S7	2.420	2.441	1.562
S8	1.825	1.732	1.316
S9	0.693	0.193	0.439
S10	1.146	0.214	0.462
S11	0.923	0.412	0.642
S12	1.844	1.547	1.244
S13	1.446	0.920	0.959
S14	2.540	2.953	1.719
S15	1.472	1.075	1.037

S16	1.657	1.226	1.107
S17	1.639	1.352	1.163
S18	1.446	0.688	0.829
S19	1.405	1.035	1.017
S20	1.858	1.165	1.079
S21	1.118	0.533	0.730
S22	1.412	0.794	0.891
S23	1.465	0.856	0.925
S24	1.642	1.050	1.025
S25	1.729	1.178	1.085
S26	2.220	1.944	1.394
S27	1.065	0.677	0.823
S28	0.712	0.228	0.477
S29	2.024	1.513	1.230
S30	1.129	1.023	1.012

Table 4.3.4: *With All Ranks*

Variable	Mean	Variance	SD
S1	1.118	1.725	1.313
S2	1.065	2.115	1.454
S3	2.066	4.997	2.235
S4	4.196	17.187	4.146
S5	1.613	4.405	2.099
S6	2.689	4.173	2.043
S7	2.726	6.270	2.504
S8	1.396	2.081	1.442
S9	0.528	0.255	0.505
S10	1.041	0.482	0.694
S11	0.822	0.932	0.965
S12	1.510	2.294	1.514
S13	1.167	1.585	1.259
S14	2.768	7.954	2.820
S15	1.274	1.975	1.405
S16	1.384	2.433	1.560
S17	1.263	1.874	1.369
S18	1.264	1.688	1.299
S19	1.039	0.961	0.980
S20	1.786	1.714	1.309
S21	0.981	1.232	1.110
S22	1.220	1.596	1.263
S23	1.302	2.185	1.478
S24	1.445	2.066	1.437
S25	1.568	2.362	1.537
S26	1.918	2.361	1.537
S27	0.757	0.651	0.807
S28	0.605	0.431	0.656
S29	2.051	3.663	1.914
S30	0.701	0.902	0.950

## 4.4 Conclusion

By design, this study involved many dominated scenarios. This enabled us to test the extent to which the stakeholder preferences were consistent with a model for scenario scores based on a monotonic function of the five criteria scores. A stakeholder who prefers a dominated to a nondominated scenario is not consistent with any such model. Of course, this does not mean that such a stakeholder is inconsistent, it simply means that his/her preferences are not consistent with this type of model. In view of the large number of dominated scenarios, we may conclude that these stakeholders are broadly, though not wholly, consistent with such a monotonic model. A more complex model possibly involving other criteria or interactions of criteria might produce a better fit, but such models would be much more cumbersome in practice.

The linear model (4.2.1) is one type of monotonic model. Owing to the inconsistencies noted above it can never yield a perfect fit, but it does seem to capture the main drift of the stakeholder preferences. This means that the expected weights (Figures 4.3.1 to 4.3.5) can be used to score coastal ecosystem threat scenarios, provided their scores on the five criteria are given and scaled appropriately.



# Application to Strategic Risk Planning in Public Health<sup>1</sup>

## 5.1 Background

Prioritization of resources, assessment of cost-effectiveness of various health interventions and equitable health care are some of the most challenging policy making processes in the area of public health. Currently, relevant analyses employ a number of summary measures: Disability Adjusted Life Years (DALYs: introduced since 1993<sup>2</sup>), Quality Adjusted Life Years (QALYs: introduced since 1968<sup>3</sup>) and Life Years gained (LYs) are the most widely accepted so far. The advantages and disadvantages of those have been assessed in a number of publications (Murray and Acharya [68];[32]; Reidpath et al. [76];Robberstad [79];Ubel et al. [97]).

From the above listed summary measures we are particularly interested in DALYs as one of its most recent applications concerns their integration in risk benefit quantitative models<sup>4</sup> that join together adverse and beneficial effects of variable

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<sup>1</sup>This chapter is based on Neslo and Cooke [72]

<sup>2</sup>DALYs were introduced as a health summary measure by the World Bank in the World Health Report 1993 (as cited in Robberstad, 2005[79]).

<sup>3</sup>QALYs were first introduced by Klarman et al. (1963) as cited in Robberstad [79]

<sup>4</sup>Quality of Life – Integrated Benefit Risk Analysis: QALIBRA is a Specific Targeted Research Project coordinated by Matis of Iceland and supported by the European Commission's 6th Framework Programme, contract number FOOD-CT-2006-022957. The project began on April 1st 2006 and will run until 2009. To assess the balance between the risks and benefits associated with a particular food, they must be converted into a common measure of net health impact. Uncertainties affecting the risks and benefits cause uncertainty about the magnitude and even the direction of the net health impact. QALIBRA will develop methods that can take account of multiple risks, benefits and uncertainties and implement them in web-based software for assessing and communicating net health impacts. Further

food consumption. The calculation of DALYs summary measures depends upon elicitation of subjective valuations of burden of disease or disease stages, i.e. disease or disease stage specific disability weights<sup>5</sup>. Subjective valuations are elicited via particular methodologies<sup>6</sup> from "experts", and then they are transformed into numerical values. This transformation allows for introducing "expert" preferences into cost-effectiveness models with the view to deciding upon resource allocation. Nevertheless, one may question a number of issues when this procedure is applied to introduce peoples' preferences in social models associated with public health policy-making:

- Transparency: disability weights employed in the calculation of DALYs are commonly cited as a single number, usually the mean of the individual "expert" (transformed) valuations. As a result, any recorded variability in expert assessments is lost.
- Ability to accommodate for either personal, social, or medical changes in time: it is understandable that disability weights elicited at a particular point in time reflect peoples' knowledge and biases for each disease at the time that elicitation occurred. Personal views may change over time due to different reasons; age and personal experiences (of "experts") maybe the most important ones, but other reasons probably are contributing, for example advances in medical science. Perhaps, peoples' preferences never change, perhaps they change only slightly, perhaps they change a lot; we cannot be certain about the validity of employing elicited health states' evaluations in studies that follow years after primary elicitations took place.
- True biological meaning of the transformed numerical values: elicited subjective valuations reflect either an individual and/or a societal point of view on different disease or disease stages, but do not rank diseases or disease stages. Therefore, equal disability weights between two or more diseases or disease stages are possible. However, most probably, all people carry particular ranking preferences for different health states.

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information can be found in <http://www.qalibra.eu>. Health endpoints of adverse and beneficial effects in the QALIBRA framework are to be expressed in a common unit, specifically Disability Adjusted Life Years (DALYs).

<sup>5</sup>DALYs summary measure combines the estimated number of life years lost (YLL) to premature death and the estimated number of years lived with disability (YLD) due to a specific disease. Whereas certain parameters of the DALYs equation can be estimated via empirical data (i.e. one could estimate Years Life Lost to a disease: YLL and Years Life with a disease: YLD via epidemiological data), the remaining parameter of disability weight (wd) is subjective and elicited as valuations of the burden of different diseases by "experts". Different techniques are employed to elicit these valuations which are transformed into disability weight normalised numbers (i.e. usually in a scale from 0=perfect health to 1=death). These techniques assess either individual (i.e. Visual Analogue Scale: VAS; Standard Gamble: SG; Time Trade-Off: TTO) or societal (i.e. Person Trade-Off: PTO) preferences over different states of health (Essink-Bot et al. [19]; Schwarzinger et al. [83])

<sup>6</sup>As above.

Further to the above, the concept of DALYs has been based on a number of technical assumptions one of which refers to that rigid, single disability weights are tied with diseases regardless of social and regional differences. As a matter of fact, this was the basis of the comparability strength of DALYs among different countries. However, this assumption carries a number of flaws as diseases may have different impact on peoples' lives according to the region they live<sup>7</sup>. Consequently, its applicability as a measure of health interventions and/or public health policies is questioned, particularly when considering food health and safety policy making in a particular geographical area, that being either a city, a state, a country, or set of countries.

The current study was set to test whether it is possible to quantify the prioritization of a health state based on a Multi Criteria Decision Model. The idea behind the approach is based upon a set of assumptions:

- Each health state maybe represented as a multidimensional point in a space defined by the weights of a precisely defined set of criteria
- The population of interest owns a true distribution of the criteria weights.
- Targeted experts whose preferences are elicited comprise a representative sample of the population of interest.

The approach followed in the study elicited ranking judgments of a number of health states rather than preference weights for diseases or disease stages, therefore excluding that two health states may result to carry the same burden. Probabilistic Inversion was applied in order to infer the relative weights (i.e. importance) of the criteria for each "expert" when determining their rank order of health states. Further, the approach used these inferred weights in order to build a linear model that combines all responses from consistent experts and can be applied in order to predict weights for further, not ranked, health states.

It is anticipated that the stepwise approach followed in this study would contribute towards three areas of interest when thinking about public health priorities and policy making:

- Identifying whether certain choices would bring a difference in peoples' health towards any direction, either for the better or the worse, without producing a number that does not carry any biological meaning.
- Organizing the thoughts and preferences of "experts" in a coherent way that would be justifiable and transparent.

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<sup>7</sup>Historically, disability weights have been designed to represent the consequences of the relative severity of each disease. They can be employed in summary measures for either a descriptive, causative or evaluative use in various fields that are affiliated with public health (Essink-Bot and Bonsel, 2002). Three major studies are published so far on elicited disability weights; these concern a range of specific diseases: a) Global Burden of Disease Study (GBD) (Murray and Lopez [69]; Murray and Acharya [68]) Dutch Disability Weights Group (Stouthard et al. [87]; Melse et al. [65]) European Disability Weights Project (Essink-Bot et al. [19]; Schwarzinger et al. [83])

- Being able to foresee changes in "experts" preferences in view of changes in time, most particularly scientific and medical ones.

## 5.2 Steps for employing the model

The following steps are followed to derive a model for valuing health states and that takes into account the the three points from mentioned above in the previous section.

1. Choose the criteria that are used to evaluate population's health.
2. Define a number of health states
3. Choose a survey format to elicit the preferences over the health states from step 2 given the criteria from step one
4. Create a model based on the criteria that can recover the preferences from step 3
5. Validate the model from step 4 as mentioned in section 1.5

In the following (sub)sections we work out the first four steps and the last step is worked out in section 5.4.

### 5.2.1 Step 1 - criteria employed to characterize scenarios

The dimensions of the EQ-5D+C descriptive system (see Table 5.2.1) were defined as the criteria or attributes that characterize each health state. These criteria are measurable quantities that although they increase in a monotonic scale they are not expressed in units. Instead, criteria levels are expressed as a score on an arbitrary scale.

### 5.2.2 Step 2 - Scenarios: health states

As mentioned in introduction, this valuation study uses the extended version EQ-5D+C (see Table 5.2.1) introduced by Stouthard et al. [87]. Although the EuroQol descriptive system is non disease specific, health states can be associated with diseases and/or disease stages via the use of questionnaires filled by patients, proxies and/or physicians. Due to human variability, as well as variability in symptoms and stages of a disease, a particular disease could be associated with a number of health states[18]. The health states were the scenarios<sup>8</sup> that experts participating in the current study judged.

<sup>8</sup>Health states employed in the current study are available on request.

**Table 5.2.1:** *The extended, six dimensional version of the original EuroQol descriptive system, i.e. EQ-5D+C*

Value	Mobility	Self Care	Usual Activities	Activities	Pain Discomfort	Anxiety Depression	Cognitive Functioning
1	No problems in walking about	No problems with self care	No problems with performing usual activities (e.g. work, study, housework)		No pain or discomfort	Not anxious or depressed	No problems in cognitive functioning
2	Some problems in walking about	Some problems washing or dressing self	Some problems with performing usual activities		Moderate pain or discomfort	Moderately anxious or depressed	Moderate problems in cognitive functioning
3	Confined to bed	Unable to wash or dress self	Unable to perform usual activities		Extreme pain or discomfort	Extremely anxious or depressed	Severe problems in cognitive functioning

17 (out of possible  $3^6 = 729$ ) health states, as these are described by the extended version (i.e. EQ-5D+C) of the EuroQol system, were defined as the scenarios that experts ranked in the current study.

The set of all 17 health states are shown in table (5.2.2). The 17 scenarios are non-dominated.

**Table 5.2.2:** *Criteria Values Per Health State*

Health States	Mobility	Self Care	Usual Activities	Activities	Pain Discomfort	Anxiety Depression	Cognitive Functioning
HS1	3	2	2		1	2	1
HS2	2	1	2		2	3	1
HS3	2	1	3		2	2	1
HS4	1	1	1		2	3	2
HS5	2	2	3		1	3	2
HS6	1	1	1		3	1	2
HS7	1	1	2		2	1	2
HS8	3	1	1		1	2	2
HS9	2	1	1		2	1	2
HS10	2	2	1		3	2	1
HS11	3	3	2		1	1	1
HS12	2	3	3		1	3	1
HS13	1	3	3		1	1	2
HS14	2	2	2		2	2	1
HS15	1	1	1		2	1	3
HS16	2	2	1		1	3	3
HS17	2	2	2		1	2	3

### 5.2.3 Step 3 - Surveys layout

Nineteen experts participated in the survey and ranked all the scenarios in each group of five. A great majority (17/19) of experts, represented a panel of "non-health care professionals" defined as people with academic background but with no health care professional experience. This did not exclude any health care personal experience, however they were asked to declare this in advance. The scenarios were presented in five groups of five. Figure (5.2.1) shows the questions asked to rank the scenarios for the first group of five.

Surveys<sup>9</sup> were sent electronically to experts during October/November 2008. The survey was divided into three parts: In parts I and II experts were invited to report personal attributes (e.g. professional affiliation, gender, age), and to recognize any potential vested interests of their selves by providing a declaration of interest. In part III, experts indicated their ranking preferences over the 17 health states. These ranking preferences were the empirical data employed to produce the criteria weights.

The 17 scenarios were presented to experts in five groups of five. Therefore, scenarios overlapped among the groups; the last two in each group were repeated as the first two in the consecutive group. This design ensured that we could test experts for consistency in their results. We tested each group for dominating scenarios, i.e. scenarios for which all criteria are of higher level when compared with the rest.

An example of a question from part III, where experts were asked their preferences ranking over a subset of the 17 health states is presented by figure 5.2.1

The results of the elicitation are captured in five preference ranking matrices that are used to fit our model. The matrices for all 19 experts are shown in Tables (5.2.3,5.2.4,5.2.5,5.2.6,5.2.7).

**Table 5.2.3:** Rank preferences Group 1

Rank	1	2	3	4	5
HS 1	6	5	2	3	3
HS 2	1	7	6	4	1
HS 3	4	4	7	3	1
HS 4	8	2	3	6	0
HS 5	0	1	1	3	14

<sup>9</sup>Survey form is available on request.

**Figure 5.2.1: Questions group 1**

**GROUP I**

Health States	Description						Your Ranking
	Mobility	Self Care	Usual Activities	Pain Discomfort	Anxiety Depression	Cognitive Functioning	
HS "R"	3	2	2	1	2	1	
HS "T"	2	1	2	2	3	1	
HS "A"	2	1	3	2	2	1	
HS "O"	1	1	1	2	3	2	
HS "C"	2	2	3	1	3	2	

Please indicate the following:

When you rank a Health State as 1 it means for you that it is:

The most severe Health State of the 5	<input type="checkbox"/>
The less severe Health State of the 5	<input type="checkbox"/>

**Table 5.2.4: Rank preferences Group 2**

Rank	1	2	3	4	5
HS 4	1	5	4	8	1
HS 5	0	0	1	4	14
HS 6	4	6	4	2	3
HS 7	12	4	3	0	0
HS 8	2	4	7	5	1

**Table 5.2.5: Rank preferences Group 3**

Rank	1	2	3	4	5
HS 7	8	7	2	0	2
HS 8	0	2	11	4	2
HS 9	9	8	1	1	0
HS 10	1	0	3	9	6
HS 11	1	2	2	5	9

**Table 5.2.6:** *Rank preferences Group 4*

Rank	1	2	3	4	5
HS 10	3	6	1	4	5
HS 11	2	5	7	3	2
HS 12	0	0	2	6	11
HS 13	4	5	5	4	1
HS 14	10	3	4	2	0

**Table 5.2.7:** *Rank preferences Group 5*

Rank	1	2	3	4	5
HS 13	1	6	5	4	3
HS 14	11	4	1	1	2
HS 15	7	5	6	1	0
HS 16	0	1	2	4	12
HS 17	0	3	5	9	2



### 5.3 Step 4 - The Model

When criteria are measured by the same level of steps, as is the case in the EQ-5D+C system, the experts may think of interrelationships between the different levels if they are asked to think about criteria weights directly. Furthermore, it can not be assumed that all experts understand the levels of each criterion in the same way. To avoid such effects one should ensure that experts do not think directly about criteria weights, therefore employing a technique to derive each expert's judgment on the importance of each criterion indirectly.

In the current study we applied a random utility model, in particular a Multi Criteria Decision Model that employs probabilistic inversion to derive criteria weights based on experts' empirical data.

We used two models in the analysis. The first is the so called *unmodelled scores* where  $u_s(a_i) = u_i$  as in the IPF and PARFUM example of section 1.3.1, taking values between zero and one. The second is the linear model formulated by equation 1.4.2. An overview of the health criteria is given in figure (5.2.2). The criteria took values 1, 2, 3 and we assumed that a higher value are always worse. As a result, the health scores will take values between  $-1$  and  $-3$ .

The *unmodelled scores* can be seen as a composition of both observed and unobserved criteria and will be used as a benchmark. If we can fit the unmodelled scores, but fail to fit linear model then we know the lack of fit is due to the linear model.

The number of health states or choice alternatives used is 17 so the set of choice alternatives defined in chapter 1 is  $\mathcal{A} = \{a_1, \dots, a_{17}\}$ . The discrete choice format that we used was the ranking of five choice alternatives in five groups. The last two choice alternatives of each group overlapped with the first two choice alternatives of the subsequent group. The discrete choice problem is given as follow

$$\begin{aligned}
 \mathcal{D} &= \{D_1, \dots, D_5\} \\
 D_1 &= \{a_1, a_2, a_3, a_4, a_5\} \\
 D_2 &= \{a_4, a_5, a_6, a_7, a_8\} \\
 D_3 &= \{a_7, a_8, a_9, a_{10}, a_{11}\} \\
 D_4 &= \{a_{10}, a_{11}, a_{12}, a_{13}, a_{14}\} \\
 D_5 &= \{a_{13}, a_{14}, a_{15}, a_{16}, a_{17}\}
 \end{aligned} \tag{5.3.1}$$

The task was to find a distribution over the weights  $(\omega_1, \dots, \omega_6)$  which reproduces the distributions over the rankings.

$$\mathcal{P}(\omega_1, \dots, \omega_6 \mid u(a_{k_i}) \text{ is } j\text{-th ranked in } u(D_k)) = \frac{\#\{s \in \mathcal{S} \mid s \text{ ranks } a_{k_i} \text{ in } j\text{-th position in } D_k\}}{\#\mathcal{S}}, k = 1, \dots, 5 \tag{5.3.2}$$

If an expert ranks health state  $a_i$  above  $a_j$  in group  $k$  then we consider an expert to be inconsistent if he ranks  $a_j$  above  $a_i$  in group  $k + 1$ .

## 5.4 Step 5 - Model adequacy and Results

To assess model adequacy proceeds in four steps:

1. We first assess expert consistency.
2. After selecting a consistent subset of experts we address the question whether any apparent agreement in rankings can be ascribed to chance, in other words, we test the hypothesis that the consistent experts' rankings are drawn at random from the set of all rankings.
3. Having rejected the hypothesis of random rankings, we ask if the experts are rational in the sense of Savage. Experts' consistency is only checked for four pairs of scenarios that were assessed in two groups. We must also check whether a distribution over the utilities of the 17 health states could reproduce all the ranking probabilities. Thus, we check whether a distribution over "unmodeled utilities" can recover the ranking probabilities.
4. If the unmodelled utilities are able to recover the ranking probabilities, can they also be recovered with a distribution over the weights in an MCDM model?

The last question is of course the most interesting, but the preceding steps are also of independent interest.

### 5.4.1 Expert consistency

In paired comparisons studies, we can tabulate the number of intransitivities, or circular triads. The sampling distributions for the number of circular triads has been computed [14] and can be used to test the hypothesis that an individual expert expresses his/her pairwise preference at random. Because of the design of this discrete choice exercise, this sort of statistical test is not an option.

When the same pair of alternatives is offered to an expert twice, we could consider a preference reversal as an event with a certain probability of occurrence. In analogy with the test of intransitivity mentioned above, we could test (and hopefully reject) the null hypothesis that this probability of reversal is  $1/2$ . In the current design, there are only 4 repeated pairs, and the probability of *no* reversals on four trials on the null hypothesis is  $1/2^4 = 0.0625$ , which is slightly above the traditional rejection level of 5%. Nonetheless, we consider that the null hypothesis of random pairwise preference is rejected (at the 0.0625 level) for experts with no preference reversals. Of the 19 experts who participated in the

study, 13 consistently ranked all of the overlapping pairs of health states, thereby rejecting the random pairwise preference hypothesis. The analysis proceeds with these 13 consistent experts.

### 5.4.2 Random preference orderings

Using Kendall's coefficient of concordance  $W$  [37],[28] we also looked if the experts rankings are random in each group. If  $W$  is one, then each expert has assigned the same order to the choice alternatives. If  $W$  is zero, then there is no overall agreement among the experts, and their responses may be regarded as essentially random. Intermediate values of  $W$  indicate a greater or lesser degree of agreement among the various responses.

Let  $R(a_i, s)$  be the rank given to health state  $a_i$  by stakeholder or expert  $s$ . Then the sum of ranks given to  $a_i$  is

$$R(a_i) = \sum_s R(a_i, s) \quad (5.4.1)$$

The mean value of these sum ranks is equal to

$$\bar{R} = \frac{1}{2}m(n+1) \quad (5.4.2)$$

with  $m$  the number of experts and  $n$  the number of health states. The sum of squared deviations is defined as

$$S = \sum_{i=1}^n (R(a_i) - \bar{R})^2 \quad (5.4.3)$$

The coefficient of concordance is then equal to

$$W = \frac{12S}{m^2(n^3 - n)} \quad (5.4.4)$$

The null hypothesis that experts choose ranks at random can be tested in terms of the values for  $S$  given  $n$  and  $m$ . Friedman [28] derived a table which contains the critical values \* of  $S$  at 5% significance level, for  $n$  between 3 and 7 and  $m$  between 3 and 20. For each group we computed the values of  $S$  and  $W$ , shown in Table (5.4.1).

**Table 5.4.1:** Values of  $S$  and  $W$  for each group

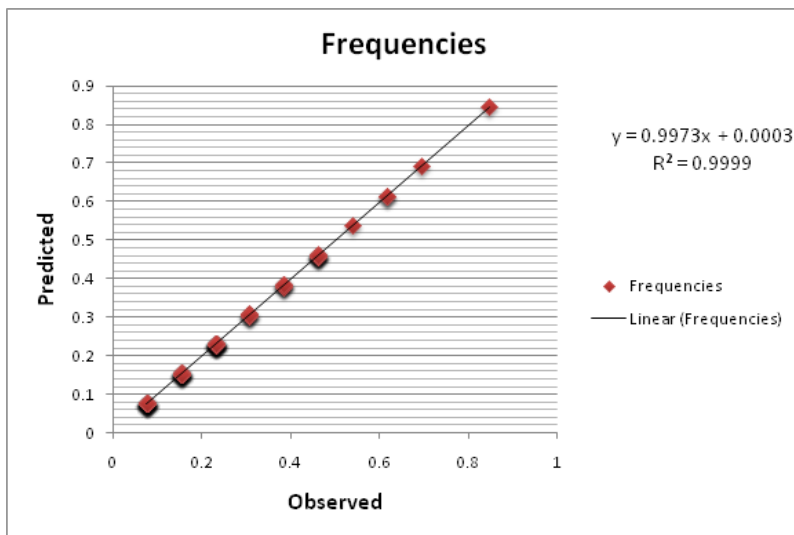
	Group 1	Group 2	Group 3	Group 4	Group 5
$S$	1166	1854	1744	1282	1597
$W$	0.323	0.514	0.483	0.355	0.443

Friedman's table does not contain the critical values for  $S$  given  $m = 19$ ; we therefore used the values for  $m = 20$ . The null hypothesis would be rejected at the 5% level for  $m = 20$  if  $S > 468.5$ . With this criterion the null hypothesis is rejected for all groups.

### 5.4.3 Savage rationality

Fitting the unmodelled scores to the data from the consistent experts yields a near perfect fit ( $R^2 = 0.999$ ), see figure 5.4.1. This means that we can assign a joint distribution over the utilities for the 17 health states, such that the probabilities of observing each health state at each rank in each  $D_k$  are predicted nearly perfectly by randomly sampling from this distribution. This merely says that our population of experts can be modeled as rational in the sense of Savage.

Figure 5.4.1: Recovery ranks consistent experts from unmodelled scores



### 5.4.4 Multi Criteria Decision Making (MCDM)

We fitted both the rank data of all experts and the rank data of the consistent experts to the MCDM model (5.4.2, 5.4.3).

Each point is an alternative-rank in each of the sets  $D_k$ . Each alternative could possibly be ranked in any of the five positions; yielding  $5 \times 5 \times 5$  points; however the actual number of points is smaller as the experts confined some alternatives to a smaller number of ranks, and zero probabilities are not plotted. The observed probabilities of rankings are on the horizontal axis, of figures 5.4.2, 5.4.3 and

Figure 5.4.2: Recovery ranks all experts

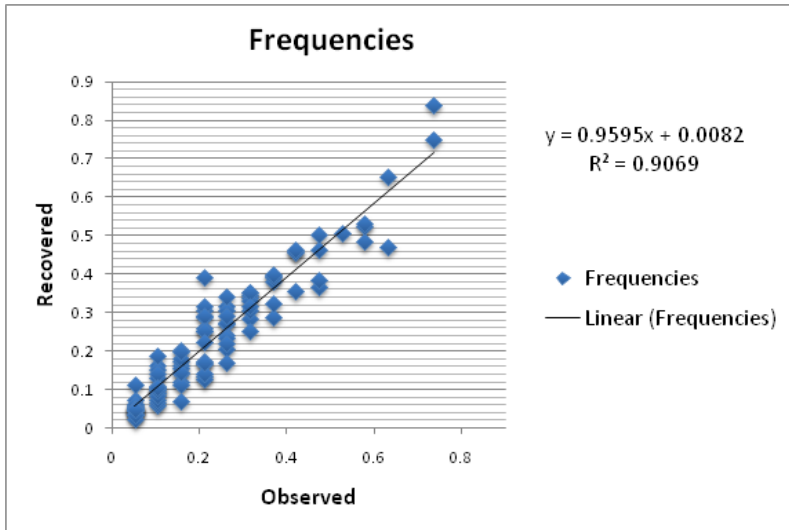
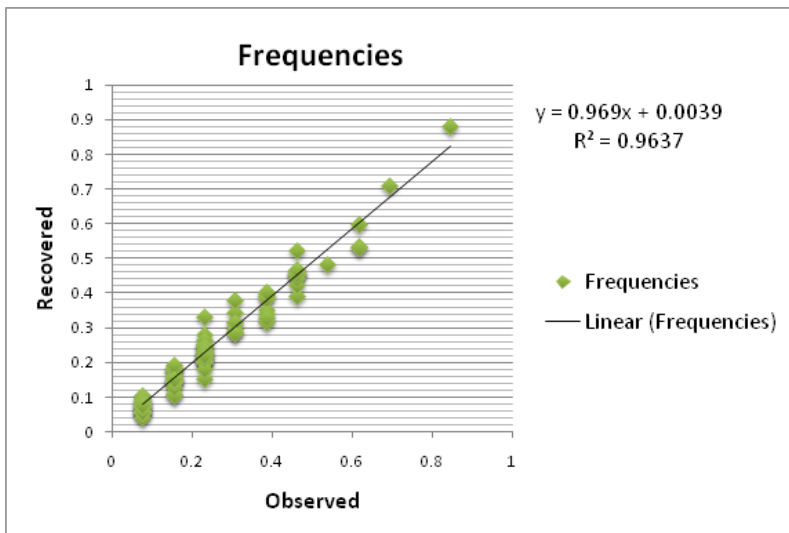


Figure 5.4.3: Recovery ranks consistent experts



the probabilities recovered by the linear model of the utilities are on the vertical axis. We used linear regression as goodness of fit measure for our method. The slope tells us how accurate the predictions are on average. And the coefficient of determination tells us how much of the variation of the observed frequencies

is explained by the predicted frequencies. Both fits have a accuracy of around 95% and a high coefficient of determination ( $R^2 = 0.906$ ), ( $R^2 = 0.964$ ) which suggests that the preferences of the experts are consistent with the linear model (1.4.2). We continue the analysis using the rankings of the consistent experts.

### 5.4.5 Criteria Weights

We fitted the model to each rank preferences groups separately to see how it affects the weights for the criteria. With the joint distribution over the weights that we obtain from fitting we can compute not only the average or mean value for each weight, but also the standard deviation and dependencies among the weights. With the standard deviation we can visualize the spread around the mean for each weight. Figures (5.4.4), (5.4.5), (5.4.6) illustrate the lower and upper bound of the spread from the weights as well as the mean values.

**Figure 5.4.4:** Subtracting one standard deviation from the mean of the weights obtained from fitting the consistent experts' rankings

Group	Mobility	Self Care	Usual Activities	Pain Discomfort	Anxiety Depression	Cognitive Functioning
1	3.62%	7.22%	3.59%	6.82%	1.80%	13.67%
2	3.26%	2.93%	0.28%	22.20%	10.28%	6.59%
3	6.49%	7.56%	6.07%	9.99%	1.65%	7.77%
4	6.23%	5.69%	2.37%	13.75%	0.24%	12.19%
5	1.60%	5.33%	2.77%	11.24%	3.37%	11.61%

**Figure 5.4.5:** Mean of the weights obtained from fitting the consistent experts' rankings

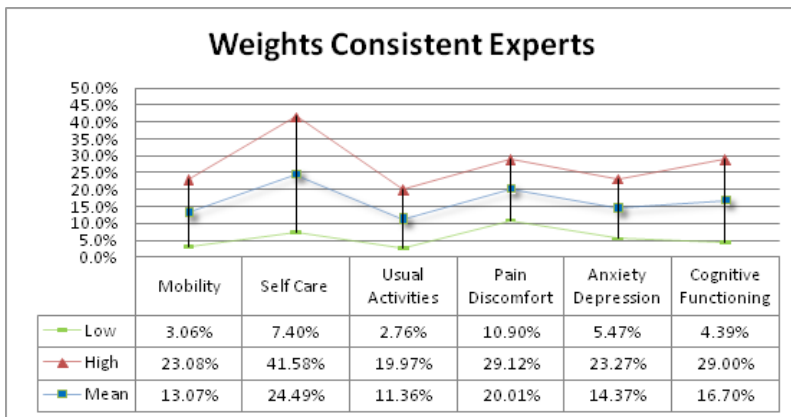
Group	Mobility	Self Care	Usual Activities	Pain Discomfort	Anxiety Depression	Cognitive Functioning
1	13.69%	18.08%	10.78%	22.53%	10.63%	24.79%
2	10.91%	11.11%	7.25%	33.10%	19.10%	18.54%
3	15.57%	17.80%	15.94%	20.08%	9.89%	20.72%
4	16.71%	15.51%	11.54%	23.96%	9.50%	22.78%
5	10.24%	14.44%	10.82%	28.27%	13.02%	23.94%

**Figure 5.4.6:** Adding one standard deviation to the mean of the weights obtained from fitting the consistent experts' rankings

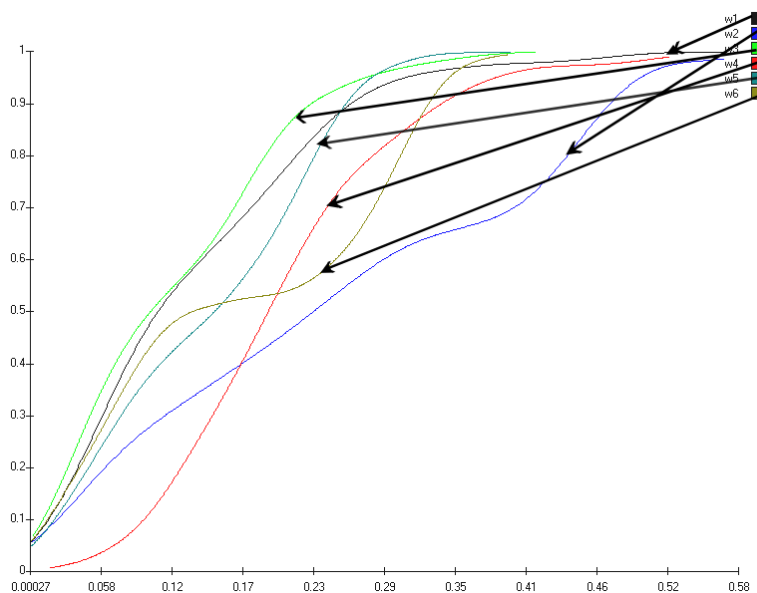
Group	Mobility	Self Care	Usual Activities	Pain Discomfort	Anxiety Depression	Cognitive Functioning
1	22.76%	28.95%	17.97%	38.24%	19.45%	35.92%
2	18.55%	19.29%	14.22%	44.00%	27.91%	30.49%
3	24.56%	28.05%	25.80%	30.17%	18.13%	33.67%
4	27.18%	25.34%	20.72%	34.17%	18.76%	33.37%
5	19.24%	23.54%	18.86%	45.30%	22.66%	34.47%

In most of the cases criterion *Pain Discomfort* is the most important factor followed by *Cognitive Functioning*, if we look at the weights obtained from fitting the rank data from each group. However if we look at the weights from fitting the rank data of all the groups we notice that criterion *Pain Discomfort* no longer is the most important factor, but *Self Care* (5.4.7).

Figure 5.4.7: Weights fitting all rank data from consistent experts



We could also read the most important criteria, fitting all the groups ,from the cumulative distribution over the weights, see figure the figure below. The cumulative distribution of the values for each weight is plotted. The most important criterion is represented by the right most distribution, which is *Self Care*.



*Cumulative Distribution of the Weights*

$w_1$	-	<i>Mobility</i>
$w_2$	-	<i>Self Care</i>
$w_3$	-	<i>Usual Activities</i>
$w_4$	-	<i>Pain Discomfort</i>
$w_5$	-	<i>Anxiety</i>
$w_6$	-	<i>Cognitive Functioning</i>

We say that the expert weights have interactions if, for example, knowledge that an expert assigns a high weight to the *Self Care* criterion gives significant information regarding weights for other criteria. Detailed analysis of interactions is not undertaken, but the correlation matrix presented in table (5.4.2) suggests that the *mobility - anxiety depression*; *self care - cognitive functioning*; *self care - usual activities*; *pain discomfort - anxiety depression* interactions are rather strong. The requirement that the weights sum to one imposes an overall negative correlation.

### 5.4.6 Health State Scores

Fitting the MCDM model not only gives us statistics about the disability weights, but also statistics about the health scores. In the introduction we mentioned that utility is affine unique, which we have used to transform the health scores to the zero one interval. Initially the health scores given the MCDM model vary



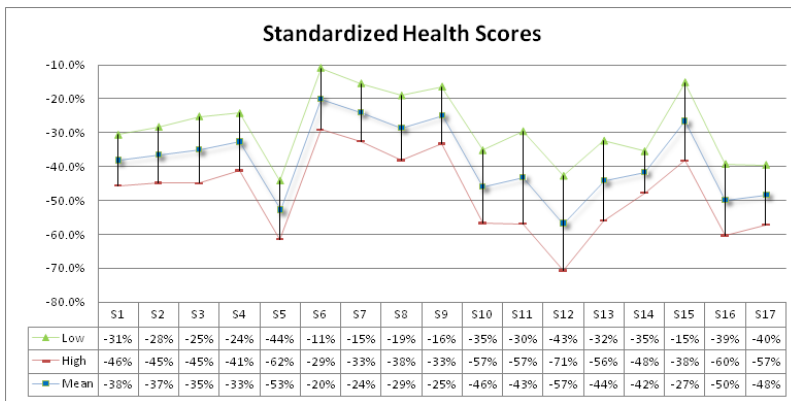
**Table 5.4.2:** Correlation coefficients of the weights.

	M	S	U	P	A	C
M	1	-0.2812	0.1018	0.1044	-0.4669	-0.1695
S	-0.2812	1	-0.5247	-0.3103	0.1577	-0.5574
U	0.1018	-0.5247	1	-0.0104	-0.0146	-0.0362
P	0.1044	-0.3103	-0.0104	1	-0.4643	-0.1107
A	-0.4669	0.1577	-0.0146	-0.4643	1	-0.1880
C	-0.1695	-0.5574	-0.0362	-0.1107	-0.1880	1

- M - Mobility
- S - Self Care
- U - Usual Activities
- P - Pain Discomfort
- A - Anxiety Depression
- C - Cognitive Functioning

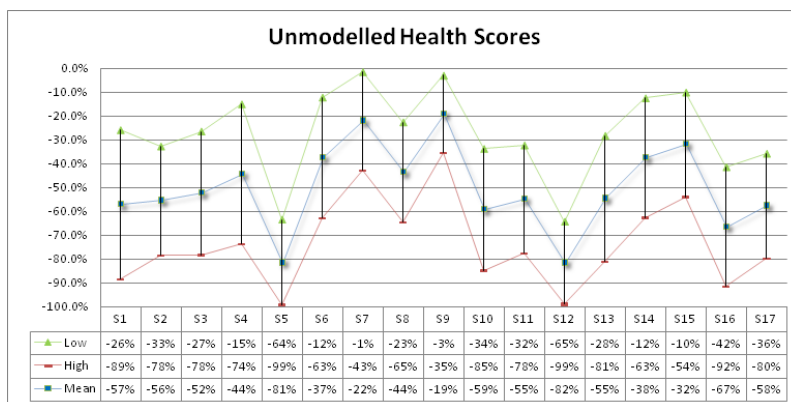
between -3 and -1, which have no tangible meaning. However if we standardize these scores we can think of them as the relative impact on health see Figure (5.4.8).

**Figure 5.4.8:** Standardized Health Scores Obtained From Fitting The Model To The Discrete Choice Data



The *unmodelled* scores presented by figure (5.4.9) are assumed to take values between -1 and 0. The variance of the *unmodelled* scores seems to be higher than the variance of the health scores from the linear model (1.4.2). Note that the ranks of the health states have slightly changed with respect to the scores from the linear model.

Figure 5.4.9: Unmodelled Health Scores



### 5.4.7 Out-of-sample validation

Finally we perform out-of-sample validation by fitting the model to a training set consisting of ranks that were attested by at least 5 experts or 38% of the experts. This model was used to predict the remaining ranks (validation set) using the fitted model. At first glance, from Figure (5.4.10) the prediction does not look good at all.

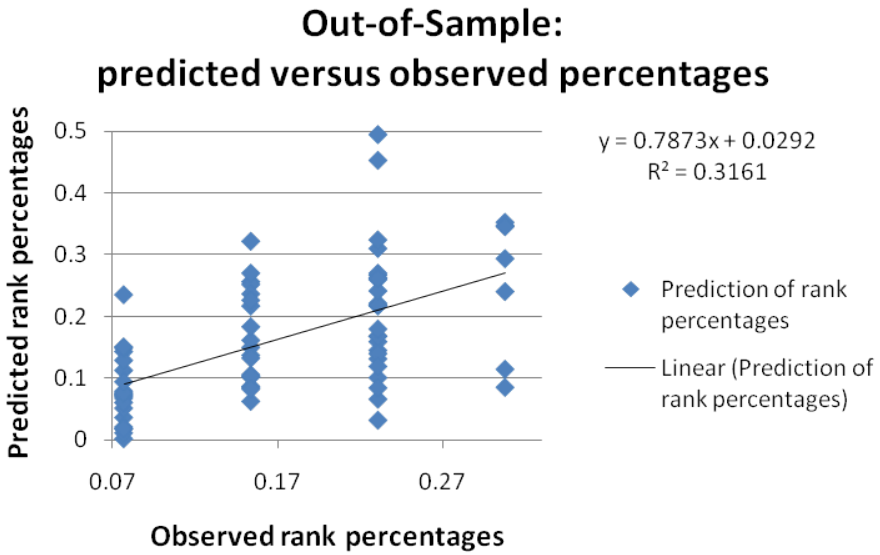
The predictions of lower ranks show very large scatter. However, if we zoom in on the ranks that got less than 38% and take the average of these predicted ranks we get a fit that is not so bad, see figure (5.4.11).

If we perform a similar out-of-sample validation using a training set of ranks that were attested by *at most* 5 experts (38% of the experts) then we get a much better fitter, see figure 5.4.12. Note that the ranks that were attested by 6 experts or not predicted accurately, but for more than 6 attestations, the predictions are quite convincing.

Performing the same exercise of averaging the predicted ranks leads to a much more overwhelming fit see figure 5.4.13.

Without undertaking an in-depth analysis, it seems that the unpopular ranks concerned primarily the lowest ranked health states, and one possible explanation for these results is that the preference judgments for the 'less important' health states were less discerning. Fitting the model to the most and least discerning leads to a different set of weights for the experts, see figures 5.4.14, 5.4.15.

**Figure 5.4.10:** Prediction of Rank Percentages Using Rank Percentages Greater Than or equal to 38%



**Figure 5.4.11:** Average Prediction of Rank Percentages Less Than 30%

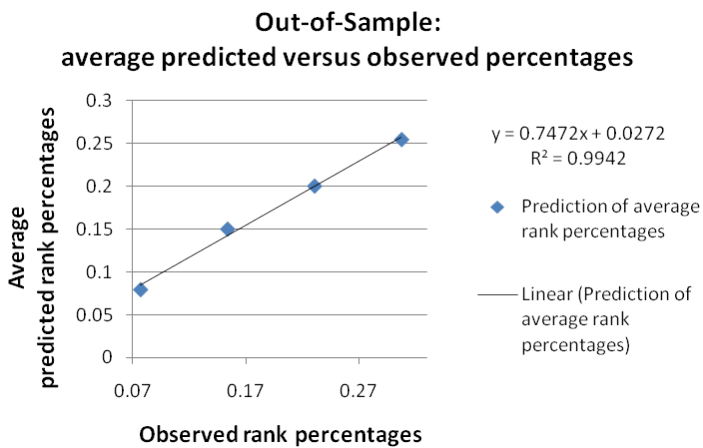


Figure 5.4.12: Prediction of Rank Percentages Using Rank Percentages Smaller Than 38%

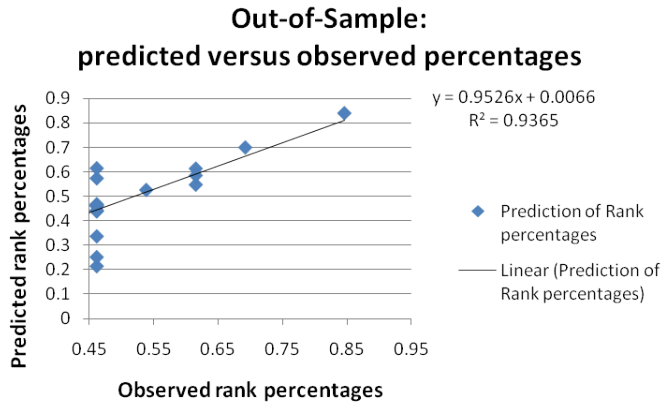


Figure 5.4.13: Average Prediction of Rank Percentages Using Rank Percentages Smaller Than 38%

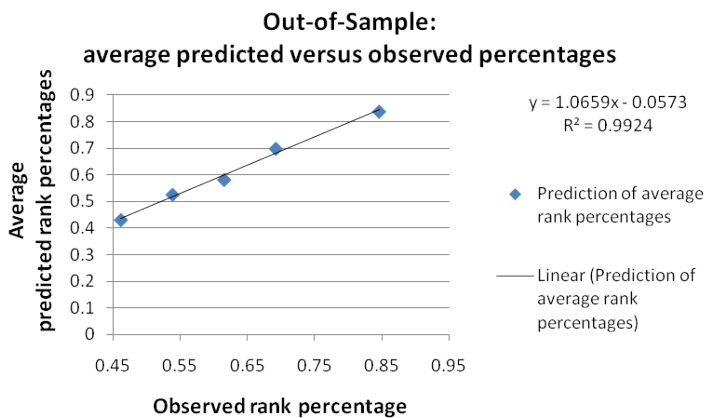


Figure 5.4.14: Weights from fitting only first ranked health states

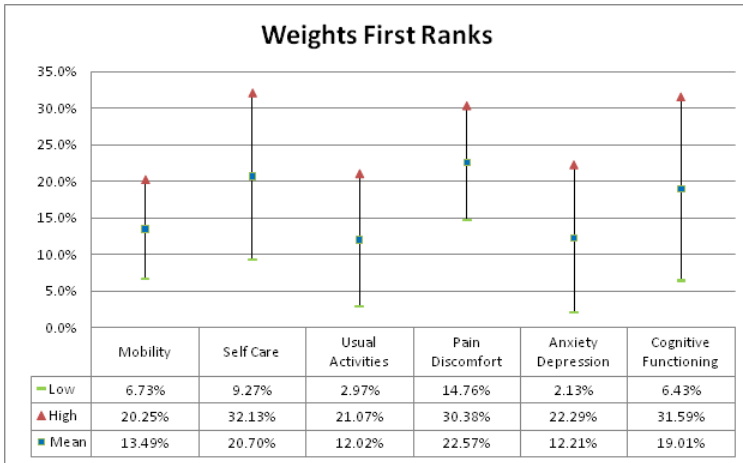
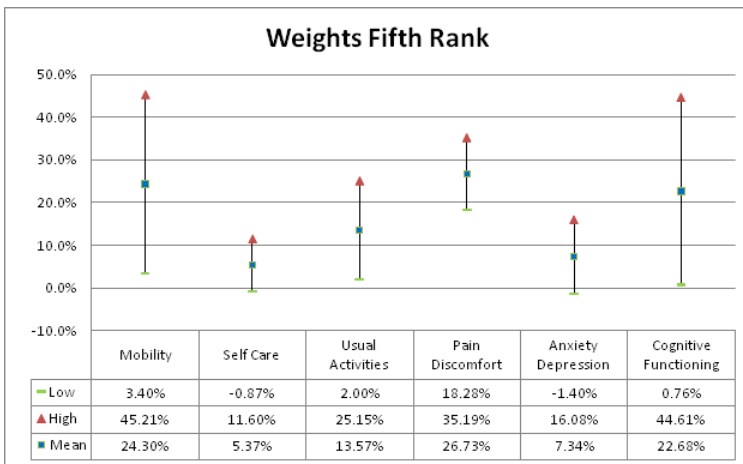


Figure 5.4.15: Weights from fitting only last ranked health states



## 5.5 Conclusion

Probabilistic inversion methods can be used to infer a distribution over utility functions based on discrete choice data. This type of application is rather new and more experience in real applications is needed. In particular, questions regarding the optimal format of the discrete choice data, the best approach to out-of-sample validation are still largely open. Equally important is how best to model utilities in terms of physical attributes. It is hoped that out-of-sample validation will eventually yield utility models with a solid scientific foundation.

# Chapter 6

## Application to The Risk Assessment of Nanotechnology Enabled Food Products<sup>1</sup>

### 6.1 Background

Research of nanotechnology has led to the development of new products and applications in the food sector. With every new advance there is the sustainability question: do the benefits outweigh the risks. The problem owner, in this case is the Food and Environment Research Agency (FERA) in the UK, was prompted by relevant research on the safety of nanotechnology enabled food products to address the risks[24].

The current state of knowledge on the safety of nanotechnology applications in the food sector still contains many gaps (EFSA<sup>2</sup>, 2009; EFSA 2011). These large knowledge gaps lead to high scientific uncertainties, and as a result they do not allow the application of standard data driven risk assessment procedures for the majority of currently developed nanotechnology applications. The problem with such approaches is that fully assessed and approved tests for the safety of nanotechnology enabled food products have yet to be developed. Even if such tests would be developed and fully certified, one would still need to overcome the hurdle of extrapolating from in vitro to in vivo. In view of this large degree of incomplete knowledge in the field of nanotechnology, an expert driven approach capturing differences in experts' opinions in a coherent way is the best alternative. The task of such an expert judgment approach would be to seek for criteria

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<sup>1</sup>This chapter is based on Flari et al. [24]

<sup>2</sup>The European Food Safety Authority

that significantly influence the safety of nanotechnology enabled food products and create a screening model based on these criteria. Morgan [67] introduced a framework for informing about the risk related to nanoparticles. This framework make use of influence diagrams based on expert judgment. These diagrams were not driven by data and merely project the relations between the criteria and safety of a food product. This model is thereby unable to screen the safety of nanoparticles.

Another approach was proposed by Linkov[53] who made use of Multi-Criteria Decision Making based on the Analytic Hierarchy Process (AHP) [80] to assess the risk of nanoparticles. AHP has a number of shortcomings[75], of which the most salient is the use of preference ratios, which presupposes a ratio scale for utilities. There is no foundation for a ratio scale, and standard utility theory defines utility values up to positive affine transformations, which of course do not preserve ratios.

Our approach makes use of the Multi-Criteria Decision Making paradigm, or more precisely Multi-Attribute Utility Theory (MAUT) [36, 21]. MAUT is mostly used to construct a utility function given multi-attributes for a single person. Because the views of multiple experts need to be captured MAUT, can not be used in it's original form. For an extension of MAUT for groups we have to direct our focus to the field of Random Utility Theory [91, 5, 78, 59, 96, 63]. Random Utility Theory or Random Utility Models derive a distribution over utility functions rather than a single utility function.

The concept of MAUT for groups is as follows:

1. identify a set of criteria that contribute significantly to the safety one wishes to assess.
2. select a number of scenarios to be ranked according to the safety of nanotechnology enabled food products, also known as alternatives.
3. determine how the scenarios score on each of the criteria.
4. identify a set of stakeholders
5. choose a survey format is chosen to elicit discrete choice preferences for the scenarios. Selection of the survey format usually depends on the number of scenarios and the questions to be answered by the study.
6. find a distribution over coefficients or weights such that the preferences of the set of experts is captured. Once such a model is found, it must be validated for its purpose.

In our study scores were calculated as a weighted linear combination of the criteria scores. As a result, the coefficients can be interpreted as the relative importance of the criteria or simply as their weights. Given a value for the weights each scenario acquires a score as a single value that can be used for ranking the



scenarios. The model that we derived is validated against all five levels mentioned in the introduction. In this study the purpose of the model was to create a screening mechanism for new products e.g. will the model mark unsafe products as unsafe and the safe products as safe. Complete validation is needed in order to test whether the model can be used as a screening model for safety of future nanotechnology-enabled food products.

Level five of validation mentioned in chapter 1 was performed at the international workshop held in the UK May 27th and 28th 2010 for experts in the field nanotechnology enabled food products organized by FERA. Experts participating at the workshop were divided in three groups and were asked to come up with a number of safe and unsafe products and fill in the criteria scores for each product. Afterwards the safety scores are computed using the distribution over the weights obtained from the model. The ranking of model is then compared to the ranking the experts gave.

The overview of this chapter is as follow. In section 6.2 we present the criteria and the model used in this study. And finally, in section 6.3 we show the result and validation of the model and show that our screening model performs reasonably using hypothetical nanotechnology enabled food products designed by a group of experts as an input.

## 6.2 Steps for employing the model

In this section we work out the six steps to employ MAUT for groups.

### 6.2.1 Step 1 - criteria employed to characterize the food products

The first step is to identify criteria that play a role in the safety of the nanotechnology enabled food products. The criteria that were identified are given in table [reftable:nanocriteria](#).

Criteria *Primary particle size*, *Secondary particle size*, *Solubility*, and *Digestibility* positively effect safety for high values and the other criteria negatively effect safety for high values.

### 6.2.2 Step 2 - scenarios: nanotechnology enabled food products

The second step is to select a number of alternatives or in our case, a number of nanotechnology enabled food products that should be appraised. In the study 26 hypothetical food products were identified by experts at FERA. These 26 hypothetical food products were constructed in such a way that there is no dominated product. No scenario is safer on all criteria, or riskier on all criteria. They resemble real applications of Nano-enabled food products, but cannot be traced back to any specific product. The scenarios are labeled from A to Z and were presented to experts in a random order to prevent ranking bias.

**Table 6.2.1:** *Criteria used in the model*

Criteria	Range	Unit	Comments
Fraction of the food	$10^{-3} - 1$	–	Criterion for exposure assessment
Fraction of the diet	0 – 100	(%)	Criterion for exposure assessment
Number of days consumed	0 – 365	<i>Days</i>	Criterion for exposure assessment
Primary particle size	$1 - 10^3$	<i>nm</i>	Criterion for hazard assessment (relating to potential absorption and translocation of ENMs from the GI tract to other parts of the body)
Secondary particle size	$1 > 10^3$	<i>nm</i>	Criterion for hazard assessment (relating to potential absorption and translocation of ENMs from the GI tract)
Surface area	6 – 200	$m^2/g$	Criterion for hazard assessment (metric for estimation of the level of potential interaction of ENMs with biological entities)
Solubility	0 – 100	(%)	Criterion for hazard and exposure assessment (relating to that fact that fully soluble materials will lose any nano-specific characteristic)
Digestibility	{ <i>Y, N</i> }	–	Criterion for hazard and exposure assessment (relating to that fact that digestible materials will lose any nano-specific characteristic)
Bio persistence	{ <i>Y, N</i> }	–	Criterion for hazard and exposure assessment (relating to that fact that non bio-persistent materials will be metabolised or excreted)
Surface modification	0 – 100	(%)	Criterion for hazard assessment (relating to the fact that surface modifications may lead to an increase or decrease in reactivity and thus potential harmful interactions)

### 6.2.3 Step 3 - Scoring matrix

The third step is to create a scoring matrix whose entries reflect how each food product performs on a particular criterion. Table 6.2.1 illustrate how each scenario scores on the different criteria.

**Table 6.2.2:** *Experts' Ranks of Nanotechnology Enabled Products*

FP	$C_1$	$C_2$	$C_3$	$C_4$	$C_5$	$C_6$	$C_7$	$C_8$	$C_9$	$C_{10}$
B	1.0E-3	3.0E+0	4.5E+1	3.0E+1	1.0E+2	2.0E+6	1.0E+1	0.0E+0	1.0E+0	2.5E+1
L	9.0E-1	5.0E+0	5.0E+1	3.0E+1	1.0E+2	2.0E+6	1.0E+2	1.0E+0	0.0E+0	0.0E+0
F	1.0E-3	1.0E+0	1.0E+1	1.0E+2	2.5E+2	6.0E+5	1.0E+1	0.0E+0	1.0E+0	5.0E+1
C	6.0E-3	5.0E+0	2.0E+2	3.0E+1	1.0E+2	2.0E+6	1.0E+1	0.0E+0	1.0E+0	0.0E+0
V	1.0E-3	2.5E+1	2.5E+1	1.0E+3	1.0E+3	6.0E+4	1.0E+1	0.0E+0	1.0E+0	1.0E+2
H	9.0E-1	4.0E+1	1.0E+1	1.0E+2	2.5E+2	6.0E+5	1.0E+2	1.0E+0	0.0E+0	5.0E+1
K	1.0E-3	1.0E+1	5.0E+1	3.0E+1	3.0E+1	2.0E+6	1.0E+1	0.0E+0	1.0E+0	5.0E+1
Z	1.0E-3	9.0E+0	3.6E+2	3.0E+1	3.0E+1	2.0E+6	1.0E+1	0.0E+0	1.0E+0	2.5E+1
Y	1.0E-2	7.0E+0	5.6E+1	1.0E+2	1.0E+2	6.0E+5	2.0E+1	0.0E+0	1.0E+0	2.5E+1
G	1.0E-3	8.0E+0	2.4E+2	1.0E+2	1.0E+2	6.0E+5	1.0E+1	0.0E+0	1.0E+0	7.5E+1
O	1.0E-3	1.5E+1	2.8E+2	1.0E+2	2.5E+2	6.0E+5	1.0E+1	0.0E+0	1.0E+0	2.5E+1
R	1.0E+0	3.0E+0	2.9E+2	3.0E+1	1.0E+2	2.0E+6	1.0E+2	1.0E+0	0.0E+0	0.0E+0

T	1.0E-3	2.0E+0	3.3E+2	1.0E+3	1.0E+3	6.0E+4	0.0E+0	1.0E+0	0.0E+0	7.5E+1
X	1.0E+0	6.0E+0	3.1E+2	1.0E+2	2.5E+2	6.0E+5	1.0E+2	1.0E+0	0.0E+0	8.0E+0
M	7.0E-3	9.0E+0	1.0E+0	1.0E+3	1.0E+3	6.0E+4	1.0E+2	1.0E+0	0.0E+0	0.0E+0
J	1.0E-3	1.0E+1	2.6E+2	1.0E+3	1.0E+3	6.0E+4	8.0E+1	1.0E+0	0.0E+0	0.0E+0
A	1.0E+0	1.4E+1	1.0E+0	3.0E+1	3.0E+1	2.0E+6	1.0E+2	1.0E+0	0.0E+0	5.0E+1
Q	1.0E-3	3.5E+0	2.0E+0	1.0E+2	2.5E+2	6.0E+5	0.0E+0	1.0E+0	0.0E+0	1.0E+2
E	8.5E-1	2.0E+0	8.0E+0	1.0E+2	1.0E+2	6.0E+5	1.0E+2	1.0E+0	0.0E+0	7.5E+1
N	1.0E-3	5.0E+0	1.8E+2	1.0E+3	1.0E+3	6.0E+4	1.0E+1	0.0E+0	1.0E+0	1.0E+2
I	9.5E-1	6.0E+0	1.9E+2	1.0E+2	1.0E+2	6.0E+5	1.0E+2	1.0E+0	0.0E+0	5.0E+1
P	1.0E-3	8.0E+0	2.8E+2	3.0E+1	1.0E+2	2.0E+6	0.0E+0	1.0E+0	0.0E+0	2.5E+1
D	1.0E+0	1.1E+1	2.4E+2	3.0E+1	3.0E+1	2.0E+6	1.0E+2	1.0E+0	0.0E+0	2.5E+1
U	1.0E-3	3.5E+1	3.0E+2	1.0E+2	2.5E+2	6.0E+5	0.0E+0	1.0E+0	0.0E+0	0.0E+0
S	5.0E-3	7.5E+0	1.5E+1	3.0E+1	1.0E+2	2.0E+6	0.0E+0	1.0E+0	0.0E+0	2.5E+1
W	5.0E-3	5.0E+0	5.0E+0	1.0E+3	1.0E+3	6.0E+4	0.0E+0	1.0E+0	0.0E+0	1.0E+2

<i>FP</i>	-	<i>Food Product</i>
<i>C</i> <sub>1</sub>	-	<i>Fraction of the food</i>
<i>C</i> <sub>2</sub>	-	<i>Fraction of the diet</i>
<i>C</i> <sub>3</sub>	-	<i>Number of days consumed</i>
<i>C</i> <sub>4</sub>	-	<i>Primary particle size</i>
<i>C</i> <sub>5</sub>	-	<i>Secondary particle size</i>
<i>C</i> <sub>6</sub>	-	<i>Surface area</i>
<i>C</i> <sub>7</sub>	-	<i>Solubility</i>
<i>C</i> <sub>8</sub>	-	<i>Digestibility</i>
<i>C</i> <sub>9</sub>	-	<i>Biopersistence</i>
<i>C</i> <sub>10</sub>	-	<i>Surface modification</i>

## 6.2.4 Step 4 - identifying and recruiting the experts

We identified and invited 53 experts all over the world with expertise on the subject matter of this study. From the 53 experts invited 26 experts accepted our invitation and 21 of these experts actually participated in the study. The backgrounds of the participating experts varied; six experts were from academia, research institutes and non-profit organizations, 3 were regulators, and 12 were governmental scientists (i.e. risk assessors, molecular biologists, toxicologists, chemists).

## 6.2.5 Step 5 - survey format

The set of responses to  $\mathcal{D}$  for all stakeholders or experts  $s \in \mathcal{S}$  is denoted by  $r_{\mathcal{D}}$  see chapter 1. In our study about nanotechnology enabled food products we had ten criteria, so we needed a larger number of food products or choicer alternatives  $\mathcal{A} = \{a_1, \dots, a_{26}\}$ , (26), from which experts could choose. As a consequence we could not rely on simple paired comparison, because people tend to slack when faced with a large number of comparisons. In this case 26 nanotechnology enabled food products would result in 325 paired comparisons. Instead, we asked experts to rank their five safest and five unsafest (riskiest) Nano-enabled food products.

## 6.2.6 Step 6 - the model

The sixth step is the representation of safety as a function of the criteria and weights. We formulated safety as a weighted linear combination of the criteria. By adopting a simple model of the utility of a food products in terms of its attribute scores, we simultaneously lighten the assessment burden and enable validation of the model. The score (utility) of food product  $i$  for stakeholder  $s$  is modeled as:

$$u_s(a_i) = \sum_{j=1}^{10} \omega_{s,j} \times c_{i,j}; \sum_{j=1}^{10} \omega_{s,j} = 1; \omega_{s,j} > 0. \quad (6.2.1)$$

where  $\omega_{s,j}$  is the weight for attribute  $j$  for stakeholder  $s$  and  $c_{i,j}$  is the score of food product  $i$  on attribute  $j$  defined by the scoring matrix in step 3. The description for the criteria used is given by table 6.2.1. In the model we've standardized the ranges of the criteria represented in table 6.2.1 to be within the zero one scale. If this model is adequate, the distribution of utility functions over the set of stakeholders may be captured as a distribution over attribute weights  $(\omega_1, \dots, \omega_{10})$ .

## 6.3 Results and Validation

We noticed a clear pattern in the experts' responses (see figure 6.3.1).

Of the 21 experts, 15 ranked food product "M" as most safe. Further, we notice that food products were rarely ranked both safe and unsafe.

### 6.3.1 Model Adequacy

A model for decision making must first be verified and validated. Both model verification and validation are performed using IPF as PI technique. Model verification is often performed by checking how well the model recovers the data. In our case the data consists of the probabilities of rankings. We used linear regression as a goodness of fit measure. The dependent and independent variables represent the observed and recovered probabilities of rankings, respectively. The slope of the regression tells how accurate the recoveries are on average, and the coefficient of determination indicates how much of the variation of the observed probabilities is explained by the recovered probabilities. We fitted the model to the safe and/or unsafe ranks and discovered that the fit of either the safe or unsafe ranks is better than the fit of all the rankings. This can be concluded from figures 6.3.1, 6.3.2, 6.3.3. This suggests that experts evaluate the criteria differently for safe and unsafe alternatives. Indeed, as shown in figures (6.3.21 and (6.3.19) the criterion solubility is weighed at 5% for the safe rankings, but becomes 10% for the unsafe rankings. Similarly, primary particle size is weighted at 12% for the safe rankings, but at 8% for the unsafe rankings. Such shifts of

**Table 6.3.1:** Experts' Ranks of Nanotechnology Enabled Products

Food Product	Rank 1	Rank 2	Rank 3	Rank 4	Rank 5	Rank 22	Rank 23	Rank 24	Rank 25	Rank 26
B	0	0	0	0	0	2	4	2	0	0
L	1	2	2	1	3	0	0	0	0	1
F	0	0	1	0	0	0	0	0	0	0
C	0	0	0	0	0	2	2	3	5	3
V	0	0	0	0	0	1	1	1	1	0
H	0	1	2	2	2	0	1	0	0	0
K	0	0	0	0	0	2	2	4	3	1
Z	0	0	0	0	0	1	1	1	6	10
Y	0	0	0	0	0	1	3	2	0	0
G	0	0	0	0	0	5	2	3	2	3
O	0	0	0	0	0	3	2	2	1	0
R	0	1	0	3	1	0	0	0	1	0
T	2	1	4	2	0	0	0	1	1	0
X	0	1	2	0	3	0	0	0	0	0
M	15	4	0	2	0	0	0	0	0	0
J	1	5	1	1	2	0	0	0	0	0
A	0	2	0	1	1	0	0	0	0	0
Q	1	2	1	1	1	1	0	0	0	0
E	0	0	3	3	0	0	0	0	0	0
N	0	0	0	0	0	1	1	1	0	1
I	0	0	0	0	3	0	0	0	0	0
P	0	0	0	0	0	1	1	0	1	0
D	0	0	0	0	1	0	0	0	0	1
U	0	0	0	1	2	1	0	1	0	1
S	0	0	1	1	1	0	1	0	0	0
W	1	2	4	3	1	0	0	0	0	0

weights are perfectly consistent with Savage rationality, but cannot be captured by simple MAUT or MCDM models.

Model validation checks the predictive ability of the model. This is also called *out-of-sample validation*. In an ideal setting we would have access to a large amount of discrete choice data. In this situation we would have a set of training data used to fit the model and a set of validation data to evaluate the model. Unfortunately when experts' input is used this isn't the case. In these situation existing data is split into a set of training data and test data. The best or optimal split of the data is still unknown and should be figured out for each application.

In this research we looked three possible splits or validation strategies namely:

1. Strategy 1 - the training set consists of ranks (both safe and unsafe) attested by more than two experts and the validation set consists of the ranks attested by one or two experts
2. Strategy 2 - the rank data (both safe and unsafe) is ordered from the most safe rank to the most unsafe rank and is the split in to pieces. The first piece

Figure 6.3.1: Fit Safe Ranks

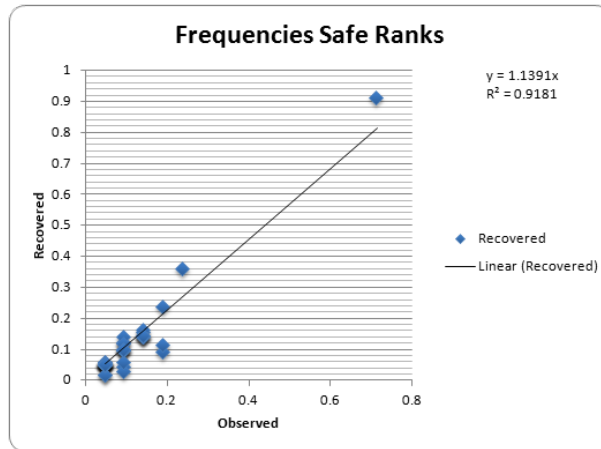
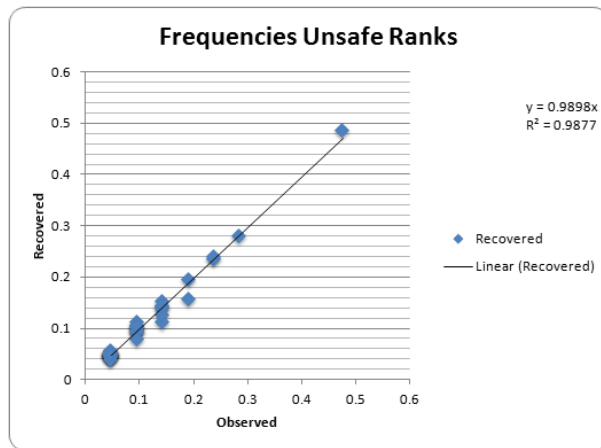


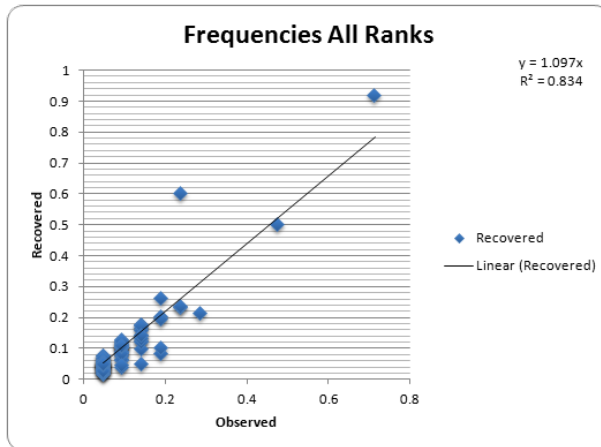
Figure 6.3.2: Fit Unsafe Ranks



of size  $2/3$ , containing the most safe ranks, is the training set. The other piece of size  $1/3$ , containing the most unsafe ranks, is the validation data

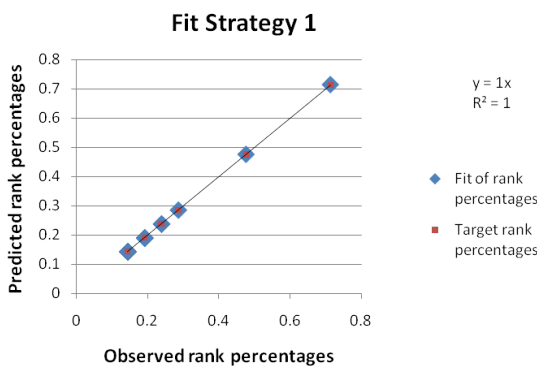
3. Strategy 3 - the rank data (both safe and unsafe) is ordered by number of experts attesting a scenario from low to high and is then split in to two pieces. The first piece of size  $2/3$ , containing the ranks with the lowest number of expert attesting, is the training set. The other piece of size  $1/3$ , containing the ranks with the highest number of expert attesting, is the validation set.

Figure 6.3.3: Fit All Ranks



The training data of strategy 1 yields a perfect fit for either the safe and/or unsafe ranks (see figure 6.3.4). There are only six dots in figure 6.3.4, because some ranks are attested by the same number of experts. Only 25 ranks that have a relative frequency higher than 0.1 were used to generate the ranks that have a relative frequency between 0 and 0.1. These 25 ranks constitute 25% of the data.

Figure 6.3.4: Fit of Rank Percentages from Strategy 1



At a first glance, the prediction of strategy 1 seems inaccurate (see figure 6.3.5). After averaging these predictions the result seem to be closer to the observed relative frequencies see (figure 6.3.6).

Figure 6.3.5: Out-of-Sample Validation Strategy 1

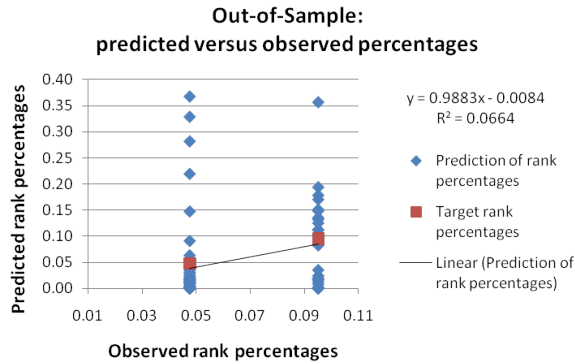
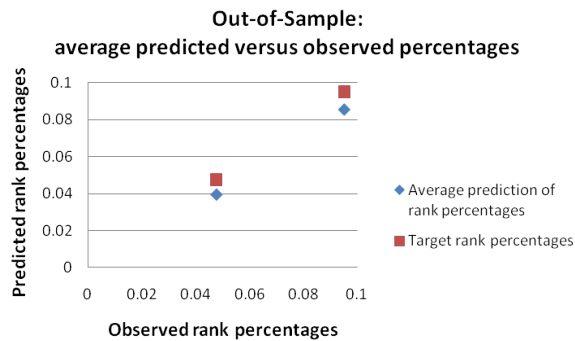


Figure 6.3.6: Out-of-Sample Validation Strategy 1 (Averaging Rank Percentages)



The training data of the strategy 2 gives a less perfect fit than the training data from the first strategy, see figure 6.3.7.

From figure 6.3.8 it follows that the second strategy has a higher coefficient of determination than the first validation strategy (figure 6.3.5), but still gives bad predictions. Averaging the prediction does not give a better picture see figure 6.3.9.

The fit of strategy 3 gives is the worst fit of them all, see figure 6.3.10. It seems that fitting the ranks that were attested by less than three experts is a problem for the PI method used. It would be strongly advised not to use this strategy for predictions, because it did not fit the training data.

The last out-of-sample validation gives a much better prediction compared with the previous strategies, see figures 6.3.11, 6.3.12.



Figure 6.3.7: Fit of Rank Percentages from Strategy 2



Figure 6.3.8: Out-of-Sample Validation Strategy 2

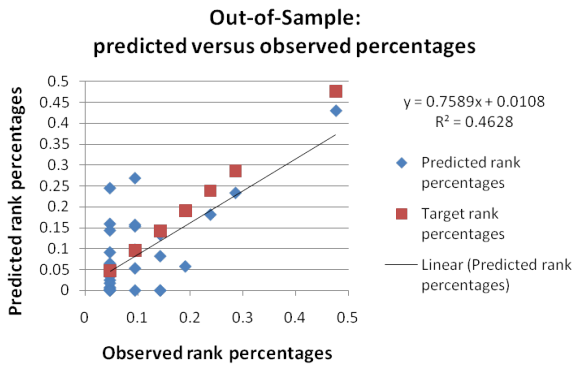


Figure 6.3.12: Out of Sample Validation Strategy 3 (Averaging Rank Percentages)

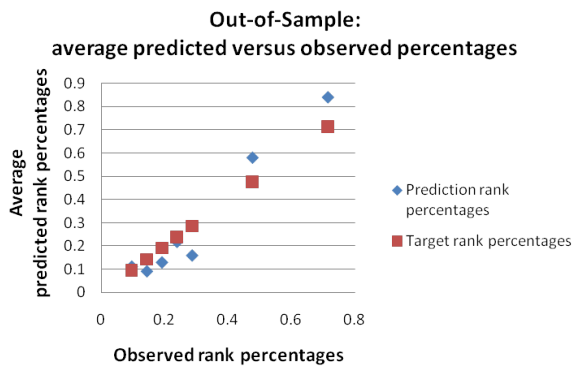


Figure 6.3.9: Out-of-Sample Validation Strategy 2 (Averaging Rank Percentages)

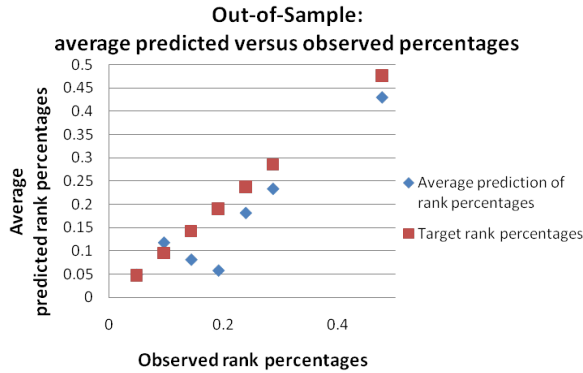
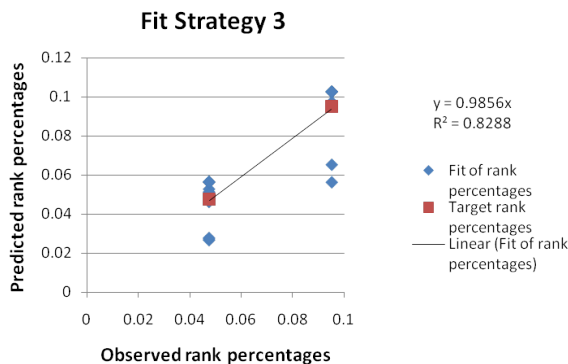


Figure 6.3.10: Fit of Rank Percentages from Strategy 3



We will use strategy 1 as our out-of-sample validation. Although it gives the worst prediction compared to strategy 2 and strategy 3 it fitted the training data perfectly.

### 6.3.2 Criteria Weights

Next we will compare the weights, scores and ranking obtained from fitting the top, bottom ranks using all the ranks as well as the ranks attested by more than two experts. From figures (6.3.13, 6.3.14, 6.3.15, 6.3.16, 6.3.17, 6.3.18) it follows that experts used different criteria assessing either safe or unsafe scenarios.

Figure 6.3.11: Out-of-Sample Validation Strategy 3

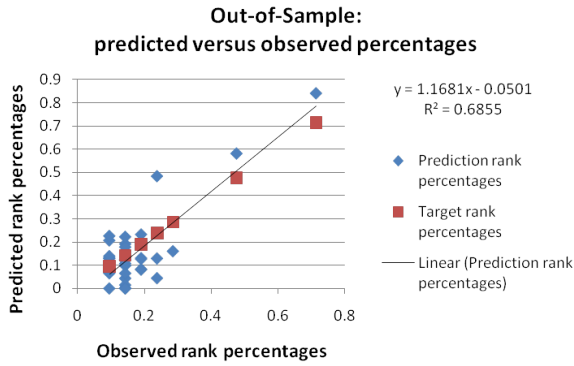
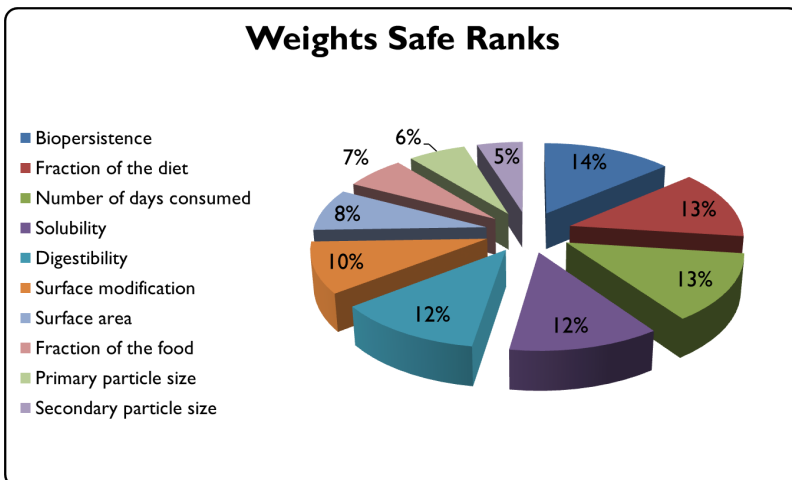
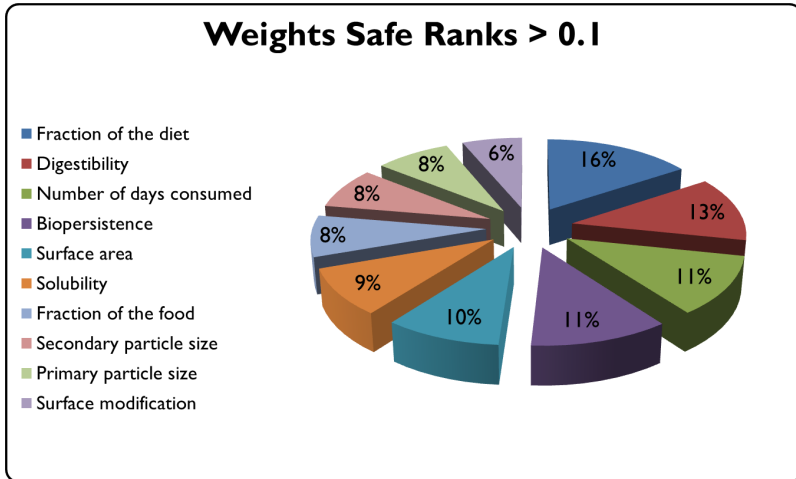


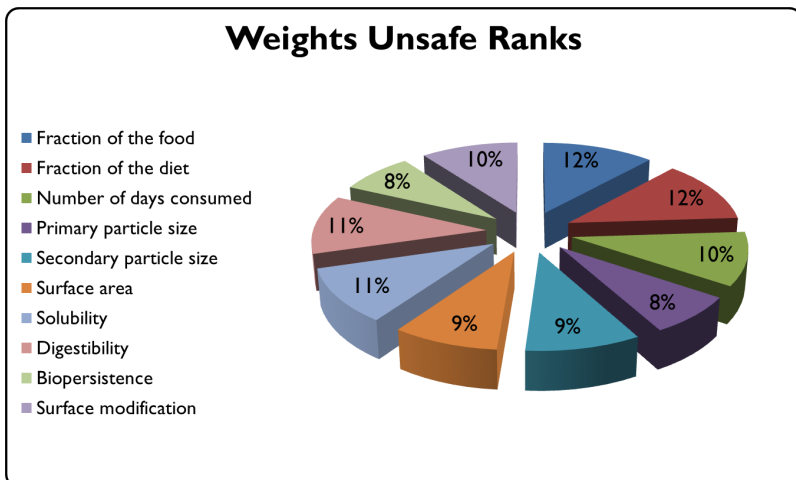
Figure 6.3.13: Weights Safe Ranks



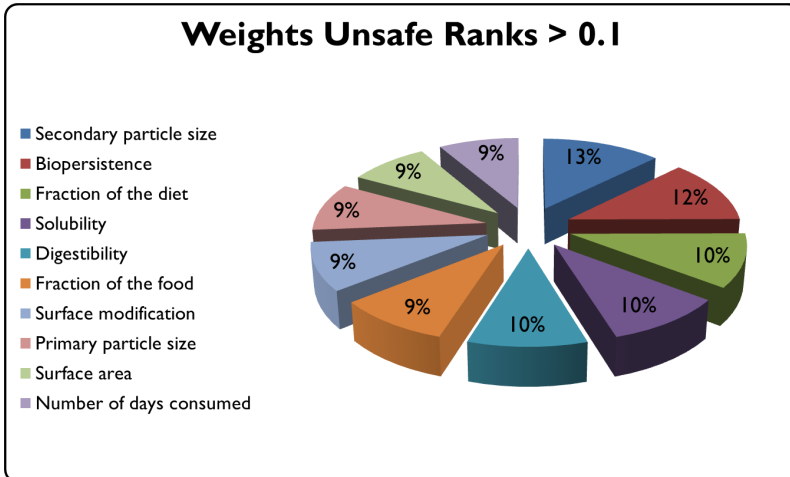
**Figure 6.3.14:** *Weights Safe Ranks Attested by More than Two Experts*



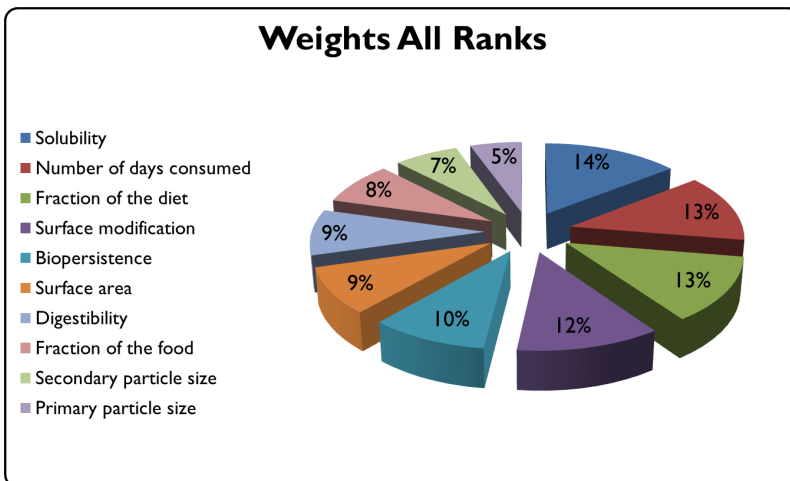
**Figure 6.3.15:** *Weights Unsafe Ranks*



**Figure 6.3.16:** *Weights Unsafe Ranks Attested by More than Two Experts*



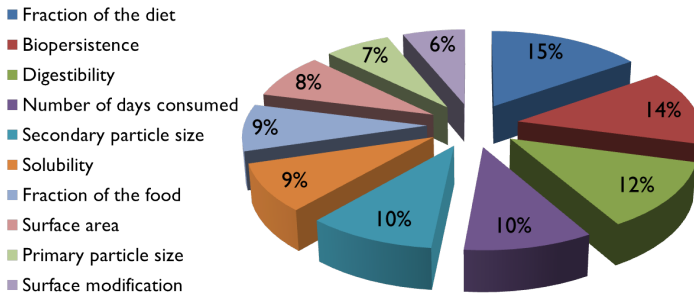
**Figure 6.3.17:** *Weights Safe and Unsafe Ranks*



We obtained complete joint distributions over the weights from which we can not only compute the average values for the weights, but also summary statistics of the distribution like the standard deviation and correlation. Figures (6.3.19, 6.3.20, 6.3.21, 6.3.22, 6.3.23, 6.3.24) illustrate the uncertainty of these weights. The low and high values are computed by subtracting and adding one standard deviation to the means of the weights, respectively. The equal weights are put in the plots to show that the weights we obtain are indeed different. Equal

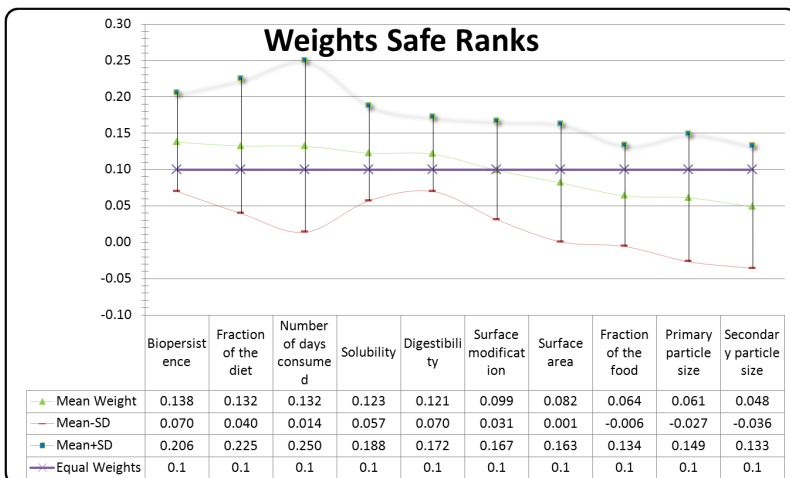
Figure 6.3.18: Weights Safe and Unsafe Ranks Attested by More than Two Experts

### Weights AI Ranks > 0.1

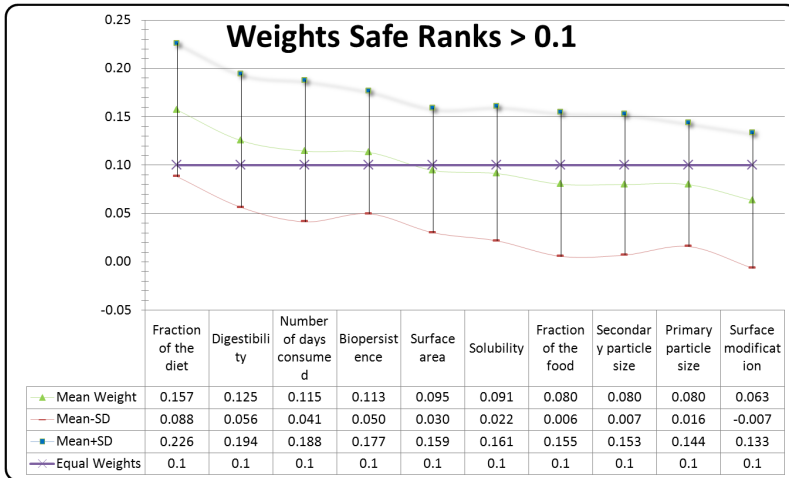


weighting will also result in a different scoring of the nanotechnology enabled food products.

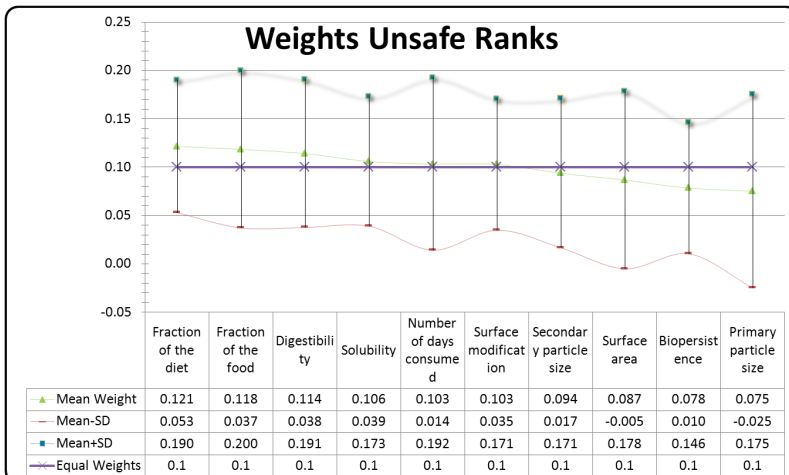
Figure 6.3.19: Mean and Standard Deviation Weights Safe Ranks



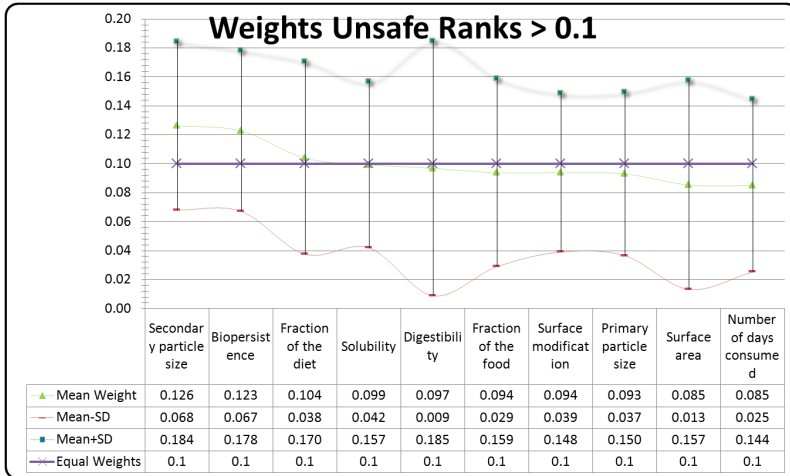
**Figure 6.3.20:** Mean and Standard Deviation Weights Safe Ranks Attested by More than Two Experts



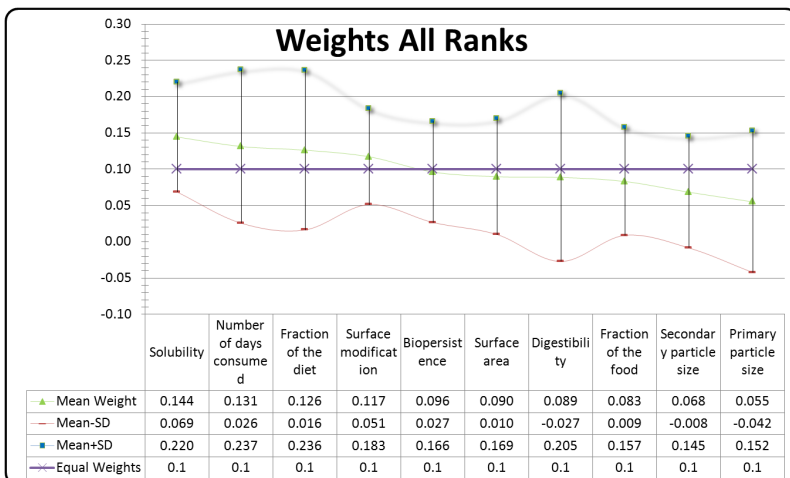
**Figure 6.3.21:** Mean and Standard Deviation Weights Unsafe Ranks



**Figure 6.3.22:** Mean and Standard Deviation Weights Unsafe Ranks Attested by More than Two Experts

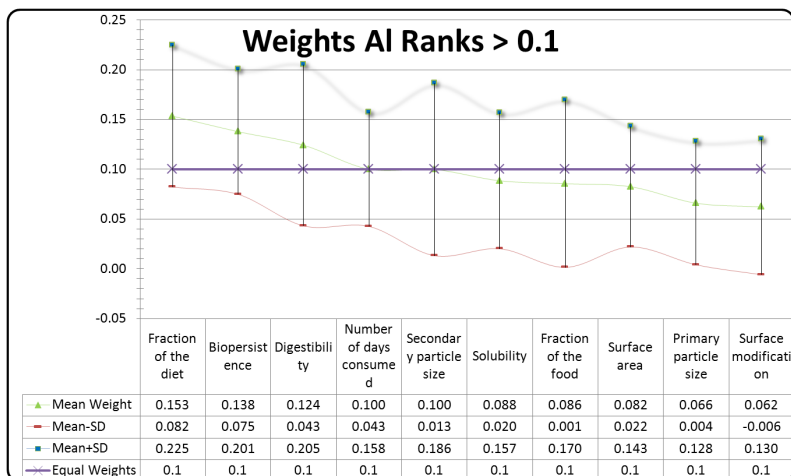


**Figure 6.3.23:** Mean and Standard Deviation Weights Safe and Unsafe Ranks





**Figure 6.3.24:** Mean and Standard Deviation Weights Safe and Unsafe Ranks Attested by More than Two Experts



To complete the analysis of the weights we present the correlation matrix from fitting all the ranks attested by more than two experts (see figure 6.3.25). Only at this fitting we found moderate positive correlation between the weights. The negative correlations are induced from the constraint that the weights have to sum up to one.

### 6.3.3 Safety Scores

The scores of the food products are also obtained from the different fittings that are presented in figures (6.3.26, 6.3.27, 6.3.28, 6.3.29, 6.3.30, 6.3.31). Notably, the top three safe food products are the same in each ranking namely, *M*, *J* and *W* and that *Z* always is the least safe.

### 6.3.4 Fresh Expert / Alternative Validation

We had the opportunity to test our model at the workshop on *Risk Assessment of Nanotechnology-enabled Food Products* organized by Dr. V. Flari<sup>3</sup>. Experts who participated at the workshop on Risk Assessment of Nanotechnology-enabled Food Products were randomly divided in three groups. These groups were asked to formulate a number of food products given the criteria we've used and record whether or not these food products are safe. These products were then plugged into the model to compute their safety score for the different fittings. After we

<sup>3</sup>Dr. V.A. Flari, Policy and Regulation Programme B, Food and Environment Research Agency, Sand Hutton, York, YO41 1LZ

Figure 6.3.25: Correlation Coefficients Weights Safe and Unsafe Ranks > 0.1

Correlation	FF	FD	NDC	PPS	SPS	SA	S	D	BP	SM
FF	1	-0.137	-0.516	0.016	0.450	-0.096	-0.602	0.039	0.188	-0.242
FD	-0.137	1	-0.013	0.048	-0.309	0.042	0.083	-0.179	-0.197	-0.082
NBC	-0.516	-0.013	1	0.039	-0.444	0.146	0.314	-0.246	-0.373	-0.011
PPS	0.016	0.048	0.039	1	-0.121	0.250	-0.316	-0.069	-0.131	-0.418
SPS	0.450	-0.309	-0.444	-0.121	1	-0.310	-0.533	0.144	0.203	-0.127
SA	-0.096	0.042	0.146	0.250	-0.310	1	-0.120	-0.175	-0.176	-0.380
S	-0.602	0.083	0.314	-0.316	-0.533	-0.120	1	-0.152	-0.193	0.356
D	0.039	-0.179	-0.246	-0.069	0.144	-0.175	-0.152	1	-0.019	-0.080
BP	0.188	-0.197	-0.373	0.203	0.203	-0.176	-0.193	-0.019	1	-0.022
SM	-0.242	-0.082	-0.011	-0.418	-0.127	-0.380	0.356	-0.080	-0.022	1

computed the scores, each group collaborated advised us whether the ordering they had in mind were preserved comparing their orderings with the orderings of the different fittings. The following table shows the results of this exercise.

The degree of external validation was less than perfect, but very substantial, although it varied according to the particular model fitting used (figure 6.3.32). The model assuming equal weights predicts correctly 6/12 of the rankings, whe-

Figure 6.3.26: Mean and Standard Deviation Scores Safe Ranks

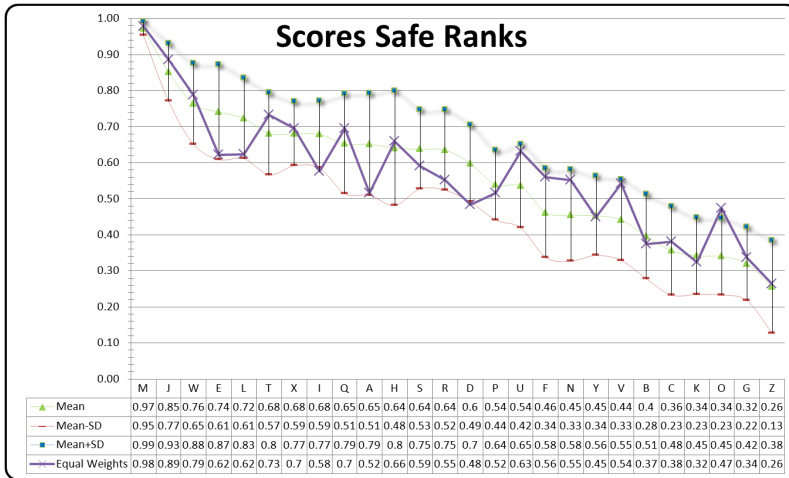
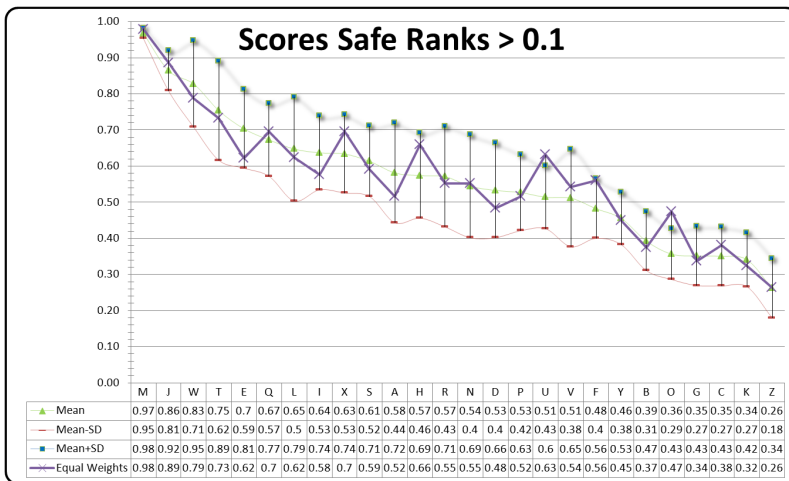


Figure 6.3.27: Mean and Standard Deviation Scores Safe Ranks > 0.1



reas the highest level of agreement, (rank order of 9/12 products correctly predicted), was achieved when the model was fitted on the experts ranking preferences of products they considered as "potentially safe".

Regardless of the model fitting and the level of agreement, the actual scores of the newly designed products from workshop participants were "clumped" within a particular scoring range. As a result, the scores did not reflect fully the degree of safety as implanted in the designed products by participants. Most probably this

Figure 6.3.28: Mean and Standard Deviation Scores Unsafe Ranks

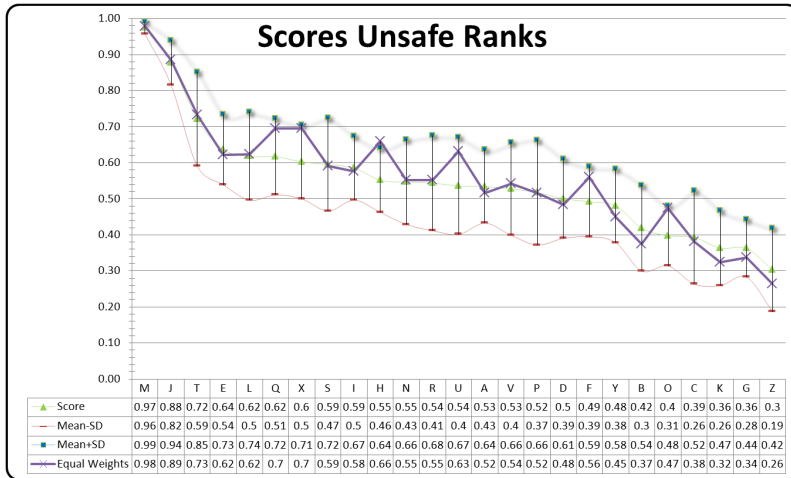
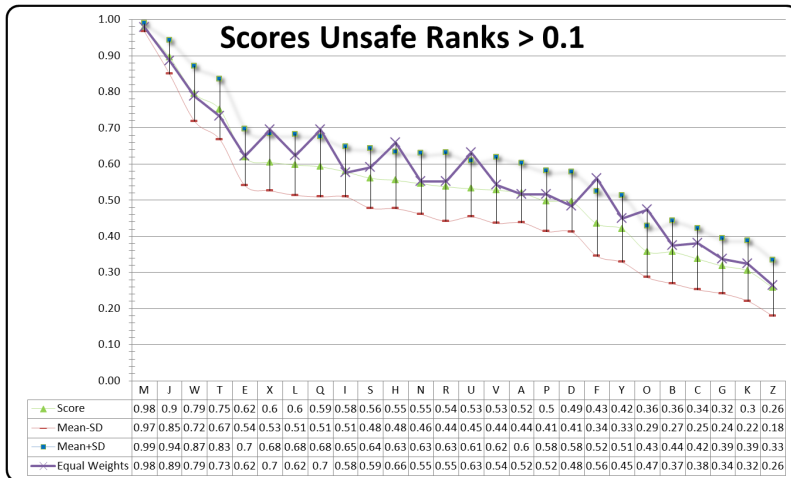


Figure 6.3.29: Mean and Standard Deviation Scores Unsafe Ranks > 0.1



happened because the model does not accommodate for particular aspects of the designed products that workshop participants took into account when designing "potentially safe" and "potentially unsafe" hypothetical products.

Figure 6.3.30: Mean and Standard Deviation Scores Safe and Unsafe Ranks

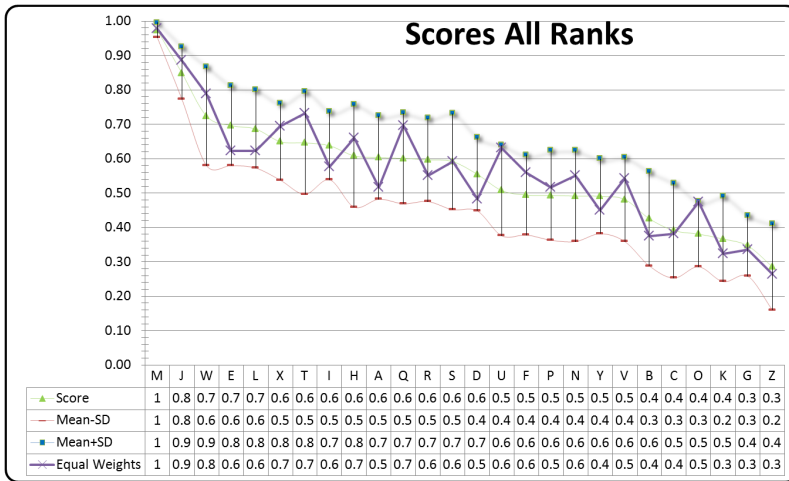


Figure 6.3.31: Mean and Standard Deviation Scores Safe and Unsafe Ranks > 0.1

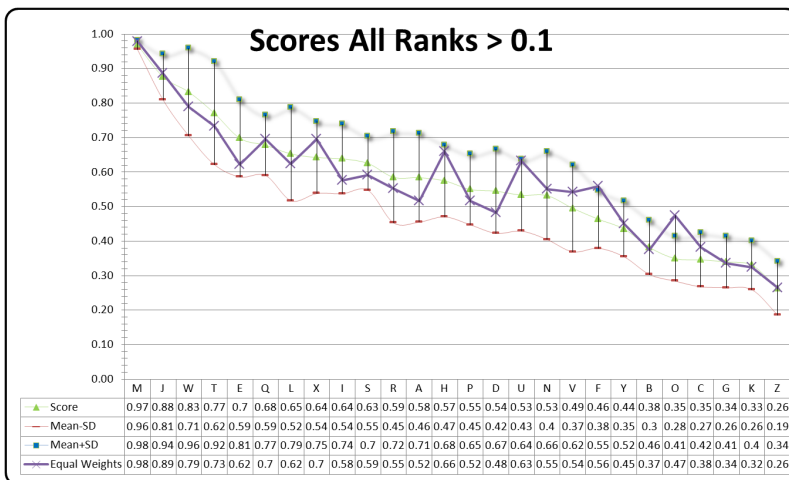


Figure 6.3.32: Expert Validation of Model

Product	Safe-All	Safe-Con.	Unsafe-All	Unsafe-Con.	(Un)Safe-All	(Un)Safe-Con.	Equal	Experts
P1G1	1	1	1	1	1	1	1	1
P2G1	2	2	2	2	2	2	2	2
P3G1	3	3	4	4	4	3	4	3
P4G1	4	4	3	3	3	4	3	4
P1G2	2	2	2	2	2	2	2	3
P2G2	1	1	1	1	1	1	1	1
P3G2	4	5	5	4	5	5	5	2
P4G2	3	3	3	3	3	3	3	4
P5G2	5	4	4	5	4	4	4	5
P1G3	2	2	2	2	2	2	2	2
P2G3	3	3	3	3	3	3	3	3
P3G3	1	1	1	1	1	1	1	1

## 6.4 Conclusions

Probabilistic inversion methods can be used to assess the safety of nanotechnology enabled food products using expert knowledge. The present application demonstrates that utility models like MCDM and MAUT can be subject to validation. We found that the MAUT model performed reasonably well in predicting results out-of-sample, and in predicting results of fresh experts and fresh alternatives. We also found that the weighting of criteria differed somewhat for safe and unsafe rankings. Although this method has been applied several times more experience with other type of applications is needed. In particular, questions regarding the optimal format of the discrete choice data, the best approach to out-of-sample validation are still largely open. Equally important is how best to model safety in terms of physical attributes. An other point that was discussed during the workshop is how often the model should be updated. This really depends on a number of factors like the rate of which new products enter the market as well information about the nano-materials. We propose an update of once per year in the near future.





## Conclusion

In this thesis we took a new approach for solving discrete choice problems. In discrete choice a distribution over utility functions is sought based on discrete choice data. Discrete choice problems are reformulated to deal with non conventional choice data and to allow for non-strict preferences in this data. Failing to distinguish between strict and non-strict preference easily leads to mis-interpretation of the results. The general advice is therefore to configure that the elicitation protocol of a discrete choice study allows stakeholders to express their indifferences, or alternatively to configure the elicitation in such a way that the possibility of indifference can be neglected.

Instead of solving discrete choice problems with conventional techniques, this thesis applies probabilistic inversion. With probabilistic inversion we infer the complete joint distribution over the utility functions without assuming a dependency structure between utility values. This is achieved by assuming a diffuse starting distribution, and adapting it iteratively to comply with the discrete choice data. Independence is often assumed as the dependency structure. This is not always appropriate, and sometimes imposes a significant "information penalty"; that is, the independence assumption can be satisfied, but only by adding significant information with respect to a non-informative distribution. And also in some situations where the dependency structure is assumed upfront might lead to no solution to the discrete choice problem even when the choice data allows for it.

With the joint distribution we can infer not only the moments and dependencies of the utility values, but also compute the probability that choice alternative  $i$  is ranked in any give position. With the insight offered by the joint distribution we were able to perform additional model validation. Typically model validation for discrete choice is performed by checking for expert consistency and checking how well the discrete choice data can be recovered or fitted by the model used. This thesis introduces further steps of validation. Not only can we fit the model if the discrete choice problem is feasible, but we can also study the predictability

capacity of the model. In other words assuming that the choice data represents the preferences of the population in question we might be able to predict stakeholders' preferences for new alternatives not present in the original data.

## 7.1 Model Validation

### 7.1.1 Consistency with Discrete Choice Data

This first step of validation is performed to check stakeholders' consistency. For the NCEAS study(chapter 4) stakeholders' consistency was checked by allowing dominated scenarios. In the health states study(chapter 5) stakeholders' consistency is checked by rank reversals. The stakeholders that had rank reversals were excluded from the study. We didn't check expert consistency for the last study presented in the thesis (chapter 6), but expert consistency could be checked as well by allowing dominated scenarios.

### 7.1.2 Consistency with Savage Rationality

Consistency with Savage rationality is checked by fitting the data to unmodeled scores. The assumption behind this validation is that when the data can fit the unmodeled scores then there exists a distribution over the utility values that satisfies the preferences.

This type of validation hasn't been carried out for the study on prioritizing marine ecosystem vulnerabilities. For the study on strategic risk planning in public health we were able to fully recover the attested ranks from the consistent experts. In case of the study on risk assessment of nano-enabled food products the we were not able to recover all the attested ranks. However when we excluded the ranks that were attested by at most 2 experts we fully recovered the remaining ranks.

### 7.1.3 In Sample Validation

With in sample validation we try to fit a MCDM or MAUT model to all attested ranks. We have not fully recovered all the attested ranks for any of the applications presented in this study. A number of reasons could cause for not fully recovering all attested ranks.

For example for the first study presented in the chapter 4 the main reason was the fact that we allowed for dominated scenarios so that we could test experts consistency. A choice alternative  $a_i$  that dominates choice alternative  $a_j$  should always be preferred to scenario  $a_j$ . Recovering preferences where scenario  $a_j$  is preferred to scenario  $a_i$  will be impossible for any model that preserves monotonicity.

In the second study represented (see chapter 6) the in sample validation was less than perfect when fitting all the attested ranks. On the other hand when fitting either the safe or unsafe attested ranks we've got far more better results. From the results of the weights we get from fitting the model to both the safe as unsafe attested ranks it follows that experts used different weights when assessing safe and unsafe products.

#### **7.1.4 Out Sample Validation**

The out of sample validation we apply is to test whether a MCDM or MAUT model used has predictability capacities. This type of validation is very new to the field of discrete choice, but seems very crucial when discrete choice models are being implemented to asses or rank other choice alternatives that were not part of the elicitation exercise. Even though we did not predict the attested ranks with perfect precision the number the overall picture seems to be that this type of validation performed moderately well. Better strategies to perform this type of validation have yet to be discovered.

#### **7.1.5 Fresh Alternative/Stakeholder Validation**

The fresh expert / alternative validation carried out in the risk assessment of nanotechnology enabled food products study(chapter 6) is new, but showed promising results. The goal of the study presented in 6 was to create a screening model based on a number of criteria. This screening model would be considered valid if it flag safe products as safe and unsafe products as unsafe. From the results of the fresh expert / alternative validation it followed that sometimes the model would mark safe products as unsafe, but the model does not flag unsafe products as safe.

## **7.2 Recommendations and Future Work**

The validation techniques proposed and applied in this thesis are not yet fully articulated, but open up opportunities to better model validation. The guiding techniques of probabilistic inversion have not been exploited to the fullest. For example we've used a moderate number of samples (around at most  $10^6$ ) for fitting the data, which is not a large number compared with current simulation models. On the other hand the number of samples can not be increased without considering a proper memory management for the PI techniques. Expressing utility as more general functions of criteria could also be explored and might lead to improved predictive performance.

Although the utility models studied in this thesis are all of the Multi Attribute Utility type, the probabilistic inversion and validation techniques are applicable

to a much wider class of utility models, involving interaction terms between criteria, non-linear functions of criteria, and "change-point models" which can switch model forms in different regions of the criteria space.

We also recommend the use of the Internet for eliciting stakeholders' preferences and communicating the results of the studies. We strongly believe that the Internet makes participating in discrete choice studies more accessible and less demanding on the stakeholders. Stakeholders can carefully express or re-enter their preferences when they see fit for as long as possible. Also when the results are available they might be able to see them and if the study allows it can also play around with the discrete data using different models.

Finally we recommend that more research should be conducted to find the optimal discrete choice format for each problem. The optimal choice of format depends on a number of things, including the number of choice alternatives, the availability of the stakeholders, and the purpose of the study. The paired comparison is well studied, but is unsuitable for modestly large numbers of choice alternatives. The alternative formats applied here, i.e. overlapping rankings and top/bottom rankings, were chosen opportunistically based on problem owner constraints. A general theory relating the discrete choice data format to the mathematical utility model to be fitted is currently unavailable.

## Software Used

The term Probabilistic Inversion (PI) has been introduced in chapter 1 as a re-sampling approach for finding a distribution over the unobserved utility values given the observed distribution over the responses and or the multi-criteria utility model. In section A.1 we give background information and an overview of the numerical methods for PI. And in section A.2 we show how the user can solve their own discrete choice problem using the software created for PI and an real life MCDM project.

### A.1 Background

The problem of inferring a random utility function  $\mathcal{P}$  from  $Q$  becomes a problem of "probabilistic inversion". Probabilistic inversion (PI) is similar to ordinary inversion. In ordinary inversion there is a function  $g$  mapping  $X$  onto  $Y$ . The value  $y^*$  is observed and the task then is to find an  $x^*$  such that  $y^* = g(x^*)$ . In the probabilistic setup the quantities  $x, y$  are random vectors instead of numbers. There are two formulations to solve a problem of probabilistic inversion namely the measure theoretic approach and the random variable approach [40] from which we choose the latter.

**Definition A.1.1.** Let  $\mathbf{X}, \mathbf{Y}$  be random vectors taking values in respectively  $\mathbb{R}^N$  and  $\mathbb{R}^M$ . Further let  $G$  be a measurable function  $G : \mathbb{R}^N \rightarrow \mathbb{R}^M$ .  $\mathbf{X}$  is called a probabilistic inverse of  $G$  at  $\mathbf{Y}$  if  $G(\mathbf{X}) \sim \mathbf{Y}$ , where  $\sim$  means "has the same distribution as". If  $\mathbf{C}$  is a set of random vectors  $\mathbf{Y}$  taking values in  $\mathbb{R}^M$ , then  $\mathbf{X}$  is an element of the probabilistic inverse of  $G$  at  $\mathbf{C}$  if  $G(\mathbf{X}) \in \mathbf{C}$ .

In case  $G = (G_1, \dots, G_M)$ , and we wish to impose marginal distributions, or marginal constraints on  $(G_1, \dots, G_M)$ , we are finding a probabilistic inverse of the set of random vectors belonging to the set  $\mathbf{C}$  satisfying the marginal constraints.

The random vectors  $\mathbf{X}$ ,  $\mathbf{Y}$  can respectively be seen as the input and the output of model  $G$ . If there exists no distribution such that  $G(\mathbf{X}) \sim \mathbf{Y}$  then we seek a random vector  $\mathbf{X}$  such that  $G(\mathbf{X})$  is 'as close as possible to'  $\mathbf{Y}$ . This will typically be achieved by minimizing the relative information  $I(G(\mathbf{X})|\mathbf{Y})$ [45]. If there is more than one probabilistic inverse of  $\mathbf{Y}$  under  $G$ , then we require a 'best' value in some suitable sense.

Probabilistic inversion problems are usually quite hopeless analytically, but there are good numerical algorithms. The key to finding a numerical solution is that we do not invert the function  $G$  at all. Instead, we begin with a diffuse initial distribution over  $\mathbb{R}^N$  such that the target distribution on  $\mathbb{R}^M$  is absolutely continuous with respect to the  $G$ -push-through of this distribution. In other words, any event which has positive probability under the target distribution must have positive mass when the initial diffuse distribution is pushed through  $G$ . We now draw a large number of samples, say  $L$ , from the initial distribution. For each sample  $(x_1, \dots, x_N)$  we compute  $G(x_1, \dots, x_N)$ . By construction, each sample has probability  $1/L$ . In general the resulting distribution of  $G$  values will not comply with the target distribution. The strategy is now to re-weight the  $L$  samples, such that if the initial distribution is re-sampled using these weights, the result does comply with the target distribution. If such a set of weights exists, the PI problem is feasible, otherwise it is infeasible. Infeasibility is hardly uncommon in these problems, and need not be serious. By minimizing infeasibility we may obtain distributions that are close to the target distribution.

There are a number of iterative methods for re-weighting an initial distribution from which we will mention two, namely IPF(Iterative Proportional Fitting)[44], [86], [20] and PARFUM (PARAmeter Fitting for Uncertainty Models)[9], [17], [50]. IPF was first described by Kruithof [44] and later rediscovered by Deming and Stephan [16], and many others. Csiszar [13] proved the convergence of IPF in case of a feasible problem. He shows that if the IPF algorithm converges, then it converges to the unique distribution (called the  $I$ -projection) which is minimally informative relative to the starting distribution, within the set of distributions satisfying the marginal constraints. PARFUM was introduced and studied by Cooke [9]. If the problem is feasible, PARFUM converges to a solution which is distinct from the IPF solution. Unlike IPF, PARFUM always converges, and it converges to a solution which minimizes a suitable information functional [17]. The convergence of PARFUM (and its canonical variations) was proved by Matus[58] but has not yet been published. When the problem is feasible IPF is preferred, because of its fast convergence. PARFUM is used when the problem is infeasible, because it insures a solution such that  $I(G(\mathbf{X})|\mathbf{Y})$  is minimal.

## A.2 User Manual

This describes how to use UNIVERSE to perform probabilistic inversion on discrete choice data in which experts choose, say, 5 top ranked scenarios from a list

of, say, 20. The scenarios are given as values on, say, 5 criteria. The functional form considered here is the standard Multi Criteria Decision Making (MCDM) format. Where  $S_k(a_i)$  is the score for scenario  $a_i$  on criteria  $k$ , the score for scenario  $a_i$  is:

$$S(a_i) = \sum_{k=1}^5 \omega_k S_k(a_i); \omega_k \geq 0; k = 1 \dots 5; \sum_{k=1}^5 \omega_k = 1 \quad (\text{A.2.1})$$

Other functional forms could be handled with equal ease, the MCDM form is chosen because it is the most familiar. Each stakeholder in a population is modeled as having his/her own specific weights  $\omega_k$ , and probabilistic inversion is used to find a distribution over the weights that recovers the experts' observed distribution over rankings of scenarios.

This is explained using a synthetic SCENRANK data set involving 20 scenarios, 124 experts, and 5 criteria, each taking values 1,2,3,4, or 5. These are nominal values whose meaning is given in narrative form, for example "very bad, bad, so?so, good, very good". In general it is preferable to have criteria in physically measurable units taking values over similar ranges. Since the "Score" is utility valued and dimensionless, the units of the weights must be "1 / criteria units".

Starting with a diffuse distribution over the weights, the goal is to find a distribution over the weights such that if our experts used a MultiCriteria Decision Model and sampled their weights from this distribution, then the probabilities of the observed rankings would be "recovered". Most importantly, we want to validate our MCDM model out of sample. That is we want to show that the model satisfactorily predicts ranking probabilities NOT used to fit the model. The SCENRANK data is in the spreadsheet

The main program is UNIVERSE developed by R. Neslo at the Department of Mathematics, Delft University of Technology. The work flow uses another program UNICORN and a graphics package UNIGRAPH. All programs can be freely downloaded from <http://risk2.ewi.tudelft.nl/oursoftware/3-unicorn>.

## 1. Transform original data to percentage rankings

Suppose you have 20 scenario's and a group of stakeholders has each ranked their top 5.

The original data may look like figure A.2.1 (from SCENRANK study, 20 scenarios, 124 experts).

Figure A.2.1: Raw Data fragment

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1																					
2	scen_rank																				
3																					
4		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
5		12543	14235	14532	15432	23145	23451	24351	25143	31254	31524	32415	35124	42315	49251	43512	45321	51234	51342	52413	54123
6	expert.nr																				
7	3	-	-	-	-	-	-	-	-	3	-	-	-	-	5	-	-	1	4	2	-
8	4	-	-	-	4	-	-	-	5	-	-	-	-	-	-	-	-	1	-	2	3
9	5	4	-	-	2	-	5	-	-	-	1	-	-	-	-	3	-	-	-	-	-
10	9	-	3	-	-	1	-	-	-	-	-	2	4	-	-	-	-	-	-	-	5
11	12	-	-	-	-	-	-	-	5	-	-	-	-	3	-	4	2	1	-	-	-
12	14	-	-	-	-	2	-	-	4	1	-	-	-	-	-	-	3	5	-	-	-
13																					
14																					

The scenarios are named  $A \dots T$ , the numbers below the scenarios are the values assigned to the 5 criteria in this study. I.e. scenario  $A$  assigns value "1" to the first criteria, "2" to the second, "5" to the third, etc. You must first transform this data to give the ranking probabilities, as shown below. This says, e.g. that 0.06504 of the 124 experts ranked scenario  $A$  in the first position (figure A.2.1).

Figure A.2.2: Rank data

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	Scenarios:																				
2		A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
3	rnk1	0.06504	0.01626	0.01626	0.04065	0.04878	0.02439	0	0	0.13821	0.17886	0.06504	0.00813	0.05691	0.03252	0.04878	0.01626	0.121951	0.06504	0.02439	0.03252
4	rnk2	0.04065	0.04065	0.03252	0.02439	0.05691	0.04878	0.00813	0	0.05691	0.14634	0.05691	0.02439	0.07317	0.02439	0.04878	0.02439	0.073171	0.0813	0.03943	0.04878
5	rnk3	0.04878	0.05691	0.04878	0.01626	0.02439	0.00813	0.04065	0.01626	0.10569	0.08943	0.06504	0.03252	0.10569	0.04878	0.04065	0.05691	0.065041	0.05691	0.06504	0.00813
6	nk4	0.07317	0.01626	0.03252	0.03252	0.05691	0.04065	0.04878	0.04878	0.07317	0.05691	0.0813	0.02439	0.10569	0.04878	0.04878	0.03252	0.056911	0.03252	0.06504	0.02439
7	rnk5	0.05691	0.04065	0.04878	0.02439	0.07317	0.06504	0.02439	0.03252	0.09756	0.06504	0.07317	0.04065	0.04065	0.04878	0.02439	0.073171	0.06504	0.05691	0.00813	
8																					

**2. Remove zeros**

A zero in the above table means that none of the 124 experts ranked scenario  $G$  in the first position, and zero's cause problems for the processing. The probability of this event is not *really* zero, we shall say that "1/2 of an expert ranked  $G$  in first place".  $(1/2) (1/124) = 0.00403$ . For the first ranked scenarios we assign probability 0.00403 to scenarios  $G$  and  $H$  and renormalize the probabilities: The first ranked variables (re-normalized) are used for the model validation, and are called *validation variables*.

**3. Define variables for fitting (training variables)**

We want to fit our model to the ranking probabilities that were attested by at least 4 of the 124 experts, NOT COUNTING the first ranks in table A.2.1. Thus the probabilities of ranking at least 0.032258. The choice of validation set is not well guided by method at this point; however one point of guidance seems to be this: don't use variables that are attested by a small number of experts as fitting



**Table A.2.1:** Renormalized probabilities

	original	re-normalized
A1	0.065041	0.064516
B1	0.01626	0.016129
C1	0.01626	0.016129
D1	0.04065	0.040323
E1	0.04878	0.048387
F1	0.02439	0.0242
G1	0	0.004032
H1	0	0.004032
I1	0.138211	0.137097
J1	0.178862	0.177419
K1	0.065041	0.064516
L1	0.00813	0.008065
M1	0.056911	0.056452
N1	0.03252	0.032258
O1	0.04878	0.048387
P1	0.01626	0.016129
Q1	0.121951	0.120968
R1	0.065041	0.064516
S1	0.02439	0.024194
T1	0.03252	0.032258

(training) or validation variables, as the results can be noisy. Once fitted, we use this model to *predict* the numbers in Table 3 – this is out-of-sample validation. Various fields of artificial intelligence refer to the variables used to fit the model as the *training set*. The training set is in table A.2.2:

#### 4. Make sample file for UNIVERSE

Universe takes as input a large sample file and changes this file to make things come out right.

In this case, we want to define a score for each scenario; for scenario A that will be:

(because A has scenario scores of (1,2,5,4,3))

Score (scenario A) =

$$\sum_{i=1}^5 w_i * S(A, i) = w_1 * 1 + w_2 * 2 + w_3 * 5 + w_4 * 4 + w_5 * 3. \quad (\text{A.2.2})$$

We must generate a large sample file of the  $w$ 's and define the scores for each scenario in each sample. Then for each scenario and each rank, we have to define an indicator variable that is 1 if that scenario has the given rank on each sample. Finally, UNIVERSE will change the sample file by re-weighting it so that the probabilities in Table 3 are realized (as close as possible). We can then check whether this re-weighted sample complies with the probabilities in the validation set (table 4).

**Table A.2.2: Fitting set**

Scenario	Experts
I2	0.0569106
K2	0.0569106
M2	0.0731707
Q2	0.0731707
R2	0.0813008
S2	0.0894309
I3	0.1056911
J3	0.0894309
M3	0.0325203
Q3	0.0569106
S3	0.0650407
A4	0.0731707
E4	0.0569106
I4	0.0731707
J4	0.0569106
K4	0.0813008
M4	0.1056911
Q4	0.0569106
S4	0.0650407
A5	0.0569106
E5	0.0731707
F5	0.0650407
I4	0.097561
J5	0.0650407
K5	0.0731707
Q5	0.0731707
R5	0.0650407

This step will require some programming, or you can use the uncertainty analysis package UNICORN to do it. Note UNICORN supports copy pasting of functions, so to make the functions shown below, it suffices to make one of each type, then copy paste it and change what needs to be changed. The unicorn file ScenRank.unc is available as an example.

First you make the random variables, these are unnormalized versions of the weights. I.e. you just make 5 uniform  $[0, 1]$  random variables. Then we specify functions of these variables, the first 5 functions convert the  $v_i$ 's to normalized weights (i.e. make them sum to one):

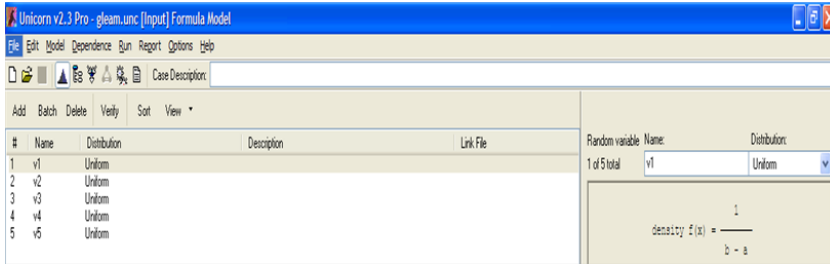
**Make weights:**

1.  $w_1 : v_1 / (v_1 + v_2 + v_3 + v_4 + v_5)$
2.  $w_2 : v_2 / (v_1 + v_2 + v_3 + v_4 + v_5)$
3.  $w_3 : v_3 / (v_1 + v_2 + v_3 + v_4 + v_5)$
4.  $w_4 : v_4 / (v_1 + v_2 + v_3 + v_4 + v_5)$
5.  $w_5 : v_5 / (v_1 + v_2 + v_3 + v_4 + v_5)$

**Define the scenario scores as in (A.2.2)**

6.  $a : 1 * w_1 + 2 * w_2 + 5 * w_3 + 4 * w_4 + 3 * w_5$

Figure A.2.3: Unnormalized versions of the weights



- 7.  $b : 1 * w_1 + 4 * w_2 + 2 * w_3 + 3 * w_4 + 5 * w_5$
- 8.  $c : 1 * w_1 + 4 * w_2 + 5 * w_3 + 3 * w_4 + 2 * w_5$
- 9.  $d : 1 * w_1 + 5 * w_2 + 4 * w_3 + 3 * w_4 + 2 * w_5$
- 10.  $e : 2 * w_1 + 3 * w_2 + 1 * w_3 + 4 * w_4 + 5 * w_5$
- 11.  $f : 2 * w_1 + 3 * w_2 + 4 * w_3 + 5 * w_4 + 1 * w_5$
- 12.  $g : 2 * w_1 + 4 * w_2 + 3 * w_3 + 5 * w_4 + 1 * w_5$
- 13.  $h : 2 * w_1 + 5 * w_2 + 1 * w_3 + 4 * w_4 + 3 * w_5$
- 14.  $i : 3 * w_1 + 1 * w_2 + 2 * w_3 + 5 * w_4 + 4 * w_5$
- 15.  $j : 3 * w_1 + 1 * w_2 + 5 * w_3 + 2 * w_4 + 4 * w_5$
- 16.  $k : 3 * w_1 + 2 * w_2 + 4 * w_3 + 1 * w_4 + 5 * w_5$
- 17.  $l : 3 * w_1 + 5 * w_2 + 1 * w_3 + 2 * w_4 + 4 * w_5$
- 18.  $m : 4 * w_1 + 2 * w_2 + 3 * w_3 + 1 * w_4 + 5 * w_5$
- 19.  $n : 4 * w_1 + 3 * w_2 + 2 * w_3 + 5 * w_4 + 1 * w_5$
- 20.  $o : 4 * w_1 + 3 * w_2 + 5 * w_3 + 1 * w_4 + 2 * w_5$
- 21.  $p : 4 * w_1 + 5 * w_2 + 3 * w_3 + 1 * w_4 + 2 * w_5$
- 22.  $q : 5 * w_1 + 1 * w_2 + 2 * w_3 + 3 * w_4 + 4 * w_5$
- 23.  $r : 5 * w_1 + 1 * w_2 + 3 * w_3 + 4 * w_4 + 2 * w_5$
- 24.  $s : 5 * w_1 + 2 * w_2 + 4 * w_3 + 1 * w_4 + 3 * w_5$
- 25.  $t : 5 * w_1 + 4 * w_2 + 1 * w_3 + 2 * w_4 + 3 * w_5$

**Define indicators for first ranked scenarios (validation variables).** The functions  $i1$  and  $i\#$  are special functions in UNICORN – if you use another program to generate samples, you’ll have to program these.  $i\#\{x,a,b,c,\dots,y\}$  returns the number of the variables  $a,\dots$  which are greater or equal to  $x$  and less or equal to  $y$ . Thus

$i\#\{0,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,a\}$

returns the number of  $b, c, \dots t$  which are  $\geq 0$  and  $\leq a$ . If this number is 19, that is equivalent to scenario  $A$  being ranked first among the 20 scenarios. This event is denoted  $a1$  and it occurs if and only if the score of  $A$  (no caps in UNICORN) as given by (1 is the highest of all 20 scores, for the particular sample of  $w$ ’s. Function number 26 below is the indicator of this event.

26.  $a1: i1\{18.5, i\#\{0,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,a\}, 19.5\}$

27.  $b1: i1\{18.5, i\#\{0,a,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,b\}, 19.5\}$

28. c1:  $i1\{18.5,i\#\{0,a,b,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,c\},19.5\}$   
 29. d1:  $i1\{18.5,i\#\{0,a,b,c,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,d\},19.5\}$   
 30. e1:  $i1\{18.5,i\#\{0,a,b,c,d,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,e\},19.5\}$   
 31. f1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,h,i,j,k,l,m,n,o,p,q,r,s,t,f\},19.5\}$   
 32. g1:  $i1\{18.5,i\#\{0,a,b,c,d,e,f,h,i,j,k,l,m,n,o,p,q,r,s,t,g\},19.5\}$   
 33. h1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,i,j,k,l,m,n,o,p,q,r,s,t,h\},19.5\}$   
 34. i\_1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i\},19.5\}$

**Unicouer doesn't allow the name i1!!!)**

35. j1:  $i1\{18.5,i\#\{0,a,b,c,d,e,f,g,h,i,k,l,m,n,o,p,q,r,s,t,j\},19.5\}$   
 36. k1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,l,m,n,o,p,q,r,s,t,k\},19.5\}$   
 37. L\_1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,m,n,o,p,q,r,s,t,l\},19.5\}$

**In courier, l (el) looks like 1 (one)**

38. m1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,n,o,p,q,r,s,t,m\},19.5\}$   
 39. n1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,o,p,q,r,s,t,n\},19.5\}$   
 40. o1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,p,q,r,s,t,o\},19.5\}$   
 41. p1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,q,r,s,t,p\},19.5\}$   
 42. q1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,r,s,t,q\},19.5\}$   
 43. r1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,s,t,r\},19.5\}$   
 44. s1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,r,t,s\},19.5\}$   
 45. t1:  $i1\{18.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,r,s,t\},19.5\}$

**Define indicators for lower ranks (training variables).**

The function  $i\#\{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i\}$  is the number of scenarios ranked below i.

$i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i\},18.5\}$

is one if and only if the rank of i is 2, i.e exactly 18 scenarios are ranked below i.

46. i2:  $i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i\},18.5\}$   
 47. k2:  $i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,l,m,n,o,p,q,r,s,t,k\},18.5\}$   
 48. m2:  $i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,n,o,p,q,r,s,t,m\},18.5\}$   
 49. q2:  $i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,r,s,t,q\},18.5\}$   
 50. r2:  $i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,s,t,r\},18.5\}$   
 51. s2:  $i1\{17.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,r,t,s\},18.5\}$   
 52. i3:  $i1\{16.5,i\#\{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i\},17.5\}$   
 53. j3:  $i1\{16.5,i\#\{0,a,b,c,d,e,f,g,h,i,k,l,m,n,o,p,q,r,s,t,j\},17.5\}$   
 54. m3:  $i1\{16.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,n,o,p,q,r,s,t,m\},17.5\}$   
 55. q3:  $i1\{16.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,r,s,t,q\},17.5\}$   
 56. s3:  $i1\{16.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,r,t,s\},17.5\}$   
 57. a4:  $i1\{15.5,i\#\{0,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,a\},16.5\}$   
 58. e4:  $i1\{15.5,i\#\{0,a,b,c,d,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,e\},16.5\}$   
 59. i4:  $i1\{15.5,i\#\{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i\},16.5\}$   
 60. j4:  $i1\{15.5,i\#\{0,a,b,c,d,e,f,g,h,i,k,l,m,n,o,p,q,r,s,t,j\},16.5\}$   
 61. k4:  $i1\{15.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,l,m,n,o,p,q,r,s,t,k\},16.5\}$   
 62. m4:  $i1\{15.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,n,o,p,q,r,s,t,m\},16.5\}$   
 63. q4:  $i1\{15.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,r,s,t,q\},16.5\}$   
 64. s4:  $i1\{15.5,i\#\{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,r,t,s\},16.5\}$

- 65. a5: i1{14.5,i#{0,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,a},15.5}
- 66. e5: i1{14.5,i#{0,a,b,c,d,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,e},15.5}
- 67. f5: i1{14.5,i#{0,a,b,c,d,e,g,h,i,j,k,l,m,n,o,p,q,r,s,t,f},15.5}
- 68. i5: i1{14.5,i#{0,a,b,c,d,e,g,f,h,j,k,l,m,n,o,p,q,r,s,t,i},15.5}
- 69. j5: i1{14.5,i#{0,a,b,c,d,e,f,g,h,i,k,l,m,n,o,p,q,r,s,t,j},15.5}
- 70. k5: i1{14.5,i#{0,a,b,c,d,e,g,f,h,i,j,l,m,n,o,p,q,r,s,t,k},15.5}
- 71. q5: i1{14.5,i#{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,r,s,t,q},15.5}
- 72. r5: i1{14.5,i#{0,a,b,c,d,e,g,f,h,i,j,k,l,m,n,o,p,q,s,t,r},15.5}

Unicorn makes 2 types of sample files <name>.sae is an Excel compliant CSV file. <name>.sam is just a single list of samples. When UNICORN is run, a sam file and a sae file are made.

A fragment of the sae file is shown below from Excel There are 167,000 samples (rows) in this case.

Figure A.2.4: Sae file from UNICORN

You can analyze the output of UNIVERSE in UNICORN by reading it back, but then you must choose the sam format (historical reasons).

**5. Read sam file into UNIVERSE.**

Open UNIVERSE, and chose the open drop down menu (figure A.2.5):

Note that we select file type sam. After choosing SCENRANK.sam we get (figure A.2.6):

The file is loaded. We have to select variables whose distribution is to be constrained to fit our expert data. That is done by choosing "variables" from the edit

Figure A.2.5: Opening Samples in UNIVERSE

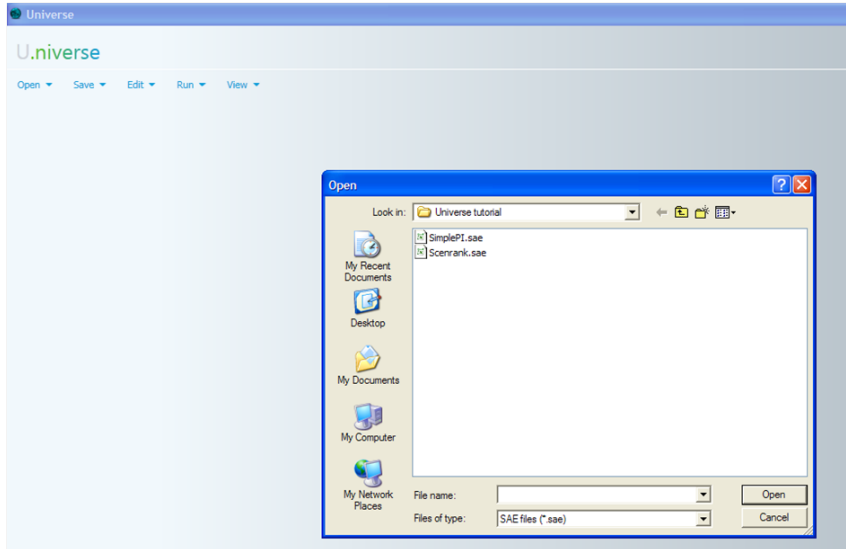
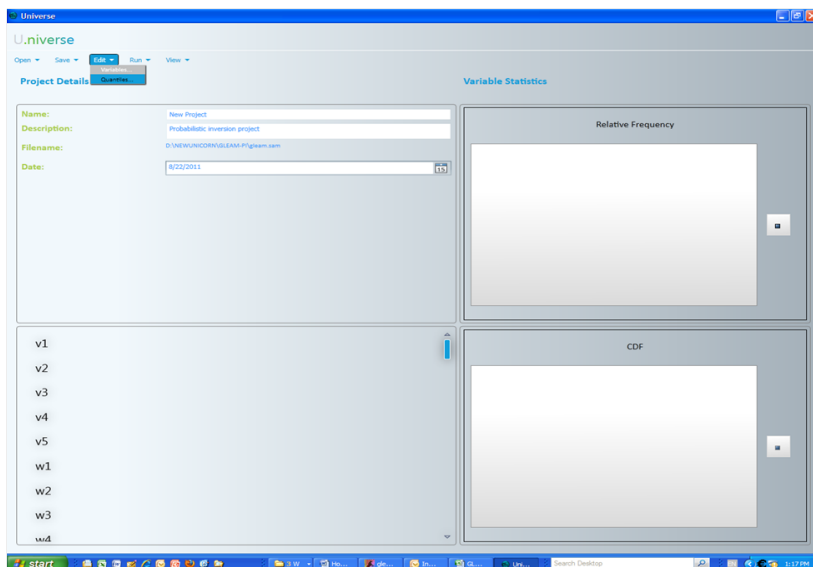
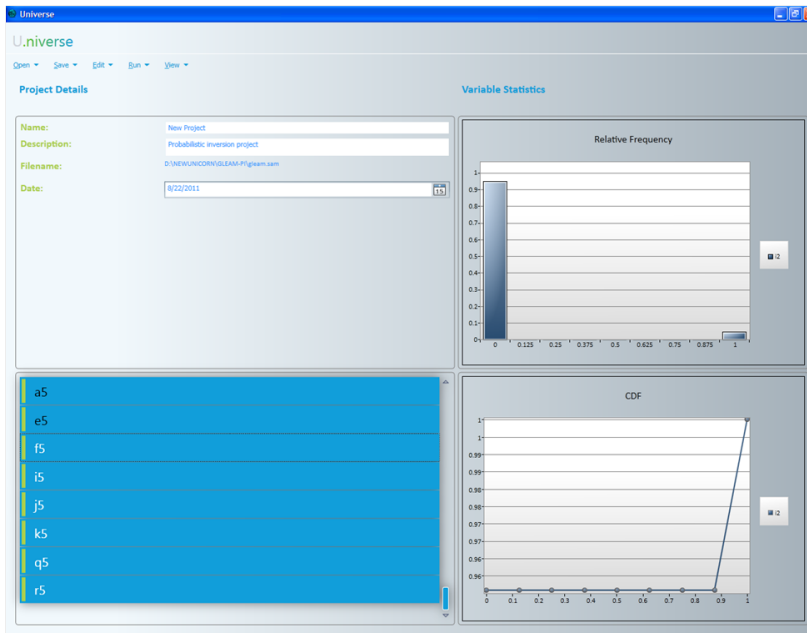


Figure A.2.6: Variables Overview UNIVERSE



menu. You select the variables with the mouse. When the set is highlighted, left click and choose "select". We select the training variables. When selected, a green bar appears as shown in figure A.2.7:

**Figure A.2.7:** Selection of Variables in UNIVERSE



Now go back to Edit and select quantiles:

On opening, it shows the minimum and maximum value of the selected variables. These variables are indicator functions, taking values 0 and 1. We want to constrain the cumulative distribution function by stipulating a number of quantiles. In case of indicators, there is only one quantile namely 0. The probability that the indicator is = 0 is 1 minus the probability we want. I.e. if we want the probability that  $A$  is ranked first to be 0.06452, then the probability of the indicator  $a_1$  being 0 must be 0.9355. In the language of UNIVERSE (which is for more general problems) the 0.9355 quantile is zero. To tell UNIVERSE that its handy to make the following columns in Excel see table A.2.3:

You can then just copy paste this information into UNIVERSE. First specify the number of quantiles, in this case 1, then hit update and you should see (figure A.2.8)

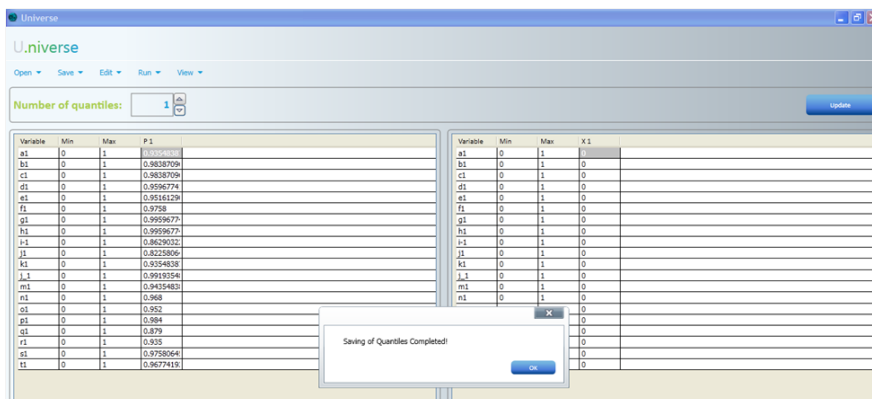
## 6. Run UNIVERSE

Go to the Run menu and select the only available option, "re-weighting". There are three re-weighting algorithms, the Default is IPF (Iterative Proportional Fitting). That will work if there IS as set of weights over the samples such that

**Table A.2.3: Handy Columns**

I2	0.056911	0.94309	0
K2	0.056911	0.94309	0
M2	0.073171	0.92683	0
Q2	0.073171	0.92683	0
R2	0.081301	0.9187	0
S2	0.089431	0.91057	0
I3	0.105691	0.89431	0
J3	0.089431	0.91057	0
M3	0.03252	0.96748	0
Q3	0.056911	0.94309	0
S3	0.065041	0.93496	0
A4	0.073171	0.92683	0
E4	0.056911	0.94309	0
I4	0.073171	0.92683	0
J4	0.056911	0.94309	0
K4	0.081301	0.9187	0
M4	0.105691	0.89431	0
Q4	0.056911	0.94309	0
S4	0.065041	0.93496	0
A5	0.056911	0.94309	0
E5	0.073171	0.92683	0
F5	0.065041	0.93496	0
I4	0.097561	0.90244	0
J5	0.065041	0.93496	0
K5	0.073171	0.92683	0
Q5	0.073171	0.92683	0
R5	0.065041	0.93496	0

**Figure A.2.8: Quantiles View UNIVERSE**



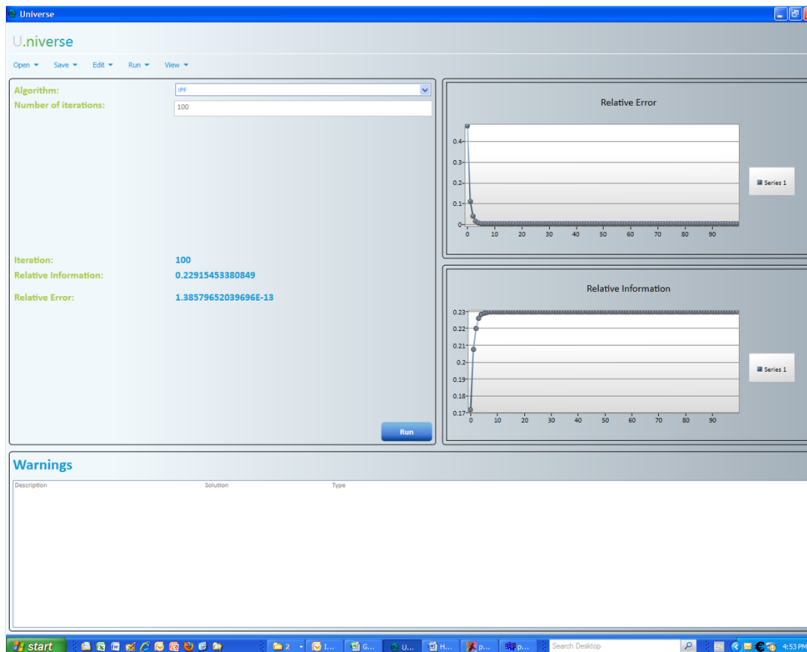
re-weighted sampling exactly recovers the required probabilities. That will not always happen. In that case the problem is infeasible – that’s not so bad, as the



"least infeasible set of weights" might be pretty good. To find that, use PARFUM. 100 iterations is usually more than enough. If the starting distribution contains no samples in one of the intervals which is constrained to have finite probability, an error message results; this is not a problem for ranked data, but in other cases, you must make sure that the numbers in the previous table are between the min and max values.

After running you see (figure A.2.9):

**Figure A.2.9:** *Simulation View Universe*



If something goes wrong you will get an error log at the bottom. The graphics show the relative information and relative error against iteration number. Relative information shows you how much the distribution is changed from the initial distribution (higher number means more change). Relative error shows the maximum of  $\langle \text{value of variable on current sample} \rangle / \langle \text{value of variable on previous sample} \rangle$ .

UNIVERSE has computed weights for each of the samples from unicorn. You can now go to VIEW and see if the probabilities after re-weighting (After probabilistic inversion, PI) agree with the stipulated weights. From the screen shot below you can see that the agreement is nearly perfect in this case (figure A.2.10).

## 7. Output from UNIVERSE

To get an output distribution from UNIVERSE we have to re-sample the initial distribution from UNICORN. Of course there is an internal version but to get an

Figure A.2.10: Probabilities Stipulated vs. Probabilities Recovered after PI

The screenshot shows the U.niverse software interface with two panels. The left panel, titled "Probabilities Stipulated", and the right panel, titled "Probabilities After PI", both display a table with two columns: "Variable" and "P 1". The data in both tables is identical, showing the following values:

Variable	P 1
a1	0.9355
b1	0.9839
c1	0.9839
d1	0.9597
e1	0.9516
f1	0.9758
g1	0.9960
h1	0.9960
i1	0.8629
j1	0.8226
k1	0.9355
j_1	0.9919
m1	0.9435
n1	0.9680
o1	0.9520
p1	0.9840
q1	0.8790
r1	0.9350
s1	0.9758
t1	0.9677

output distribution we have to stipulate how many samples we want. Go back to RUN and choose re-sampling. Stipulate the number of samples hit "sample" and then hit "save". Don't forget to save, otherwise you won't have anything. Although there were 16,000 samples in the sam file, we've chosen to sample the re-weighted file 10,000 times.

When saving you can choose the file type. For an Excel compliant CVS file, chose sae. If you wish to get the stats from UNICORN, chose sam. In either case you can get graphic output from UNIGRAPH – also free from the same website as UNICORN.

### 8. Output from UNICORN.

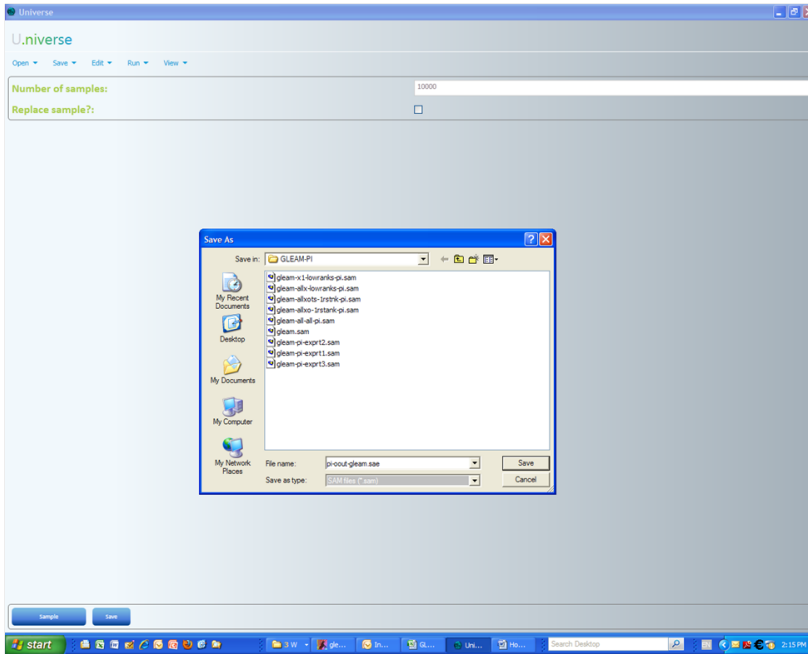
Open UNICORN (figure A.2.12) , from FILE choose "New formula Model" and choose "BATCH" (figure A.2.13), and then "create from sample file". Select the sam file just created in UNIVERSE.

If you want stats of certain variables, you have to enter them as functions of input – this is legacy. Thus if you want to compare scenarios *A*, *B* and *C*, create input *ScenA*, *ScenB*, *ScenC*, and assign these functions the values a,b,c respectively. Then run the simulation, UNICORN just takes one pass through the sample and gathers the stats for the functions. Choose output format rtf, and you can get the stats in ms word tables. Here's a screen shot (figure A.2.14):

You can also analyze the results graphically with UNIGRAPH, that easily makes cobweb plots, scatter plots and the like. Here's a cobweb plot of of the weights and scores for A,B and C (figure A.2.15).

By dragging the mouse, we can select samples which pass through certain regions. In the following all samples were selected in which *ScenB* was high. We see that in that case *ScenA* and *ScenB* are relatively low and weight  $w_2$  has to be rather

Figure A.2.11



high (figure A.2.16).

Figure A.2.12: New UNICORN File

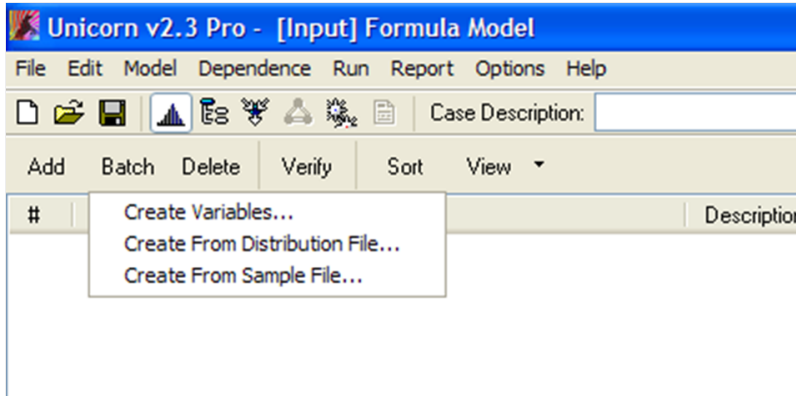


Figure A.2.13: Batch Create Variables

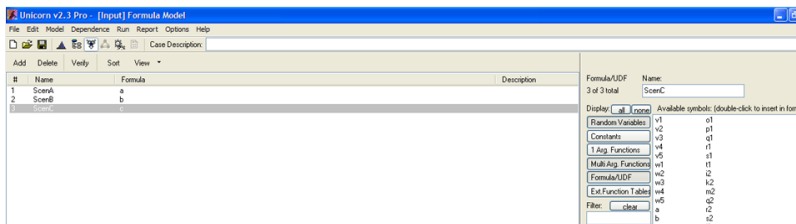


Figure A.2.14: Summary Statistics of the Variables in UNICORN

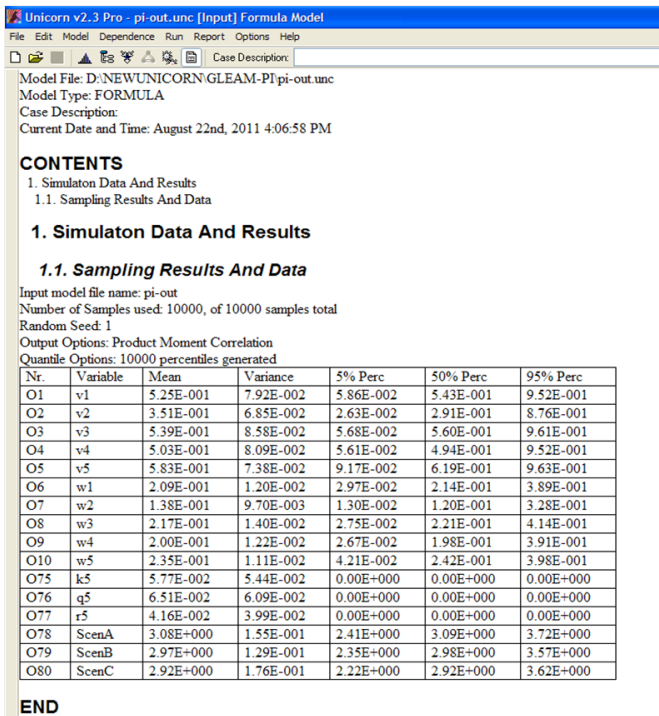
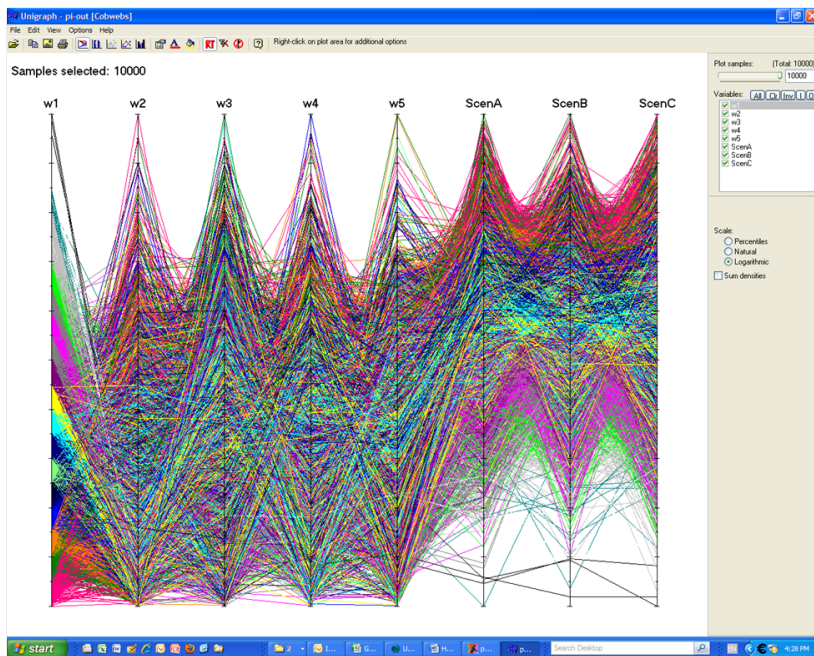
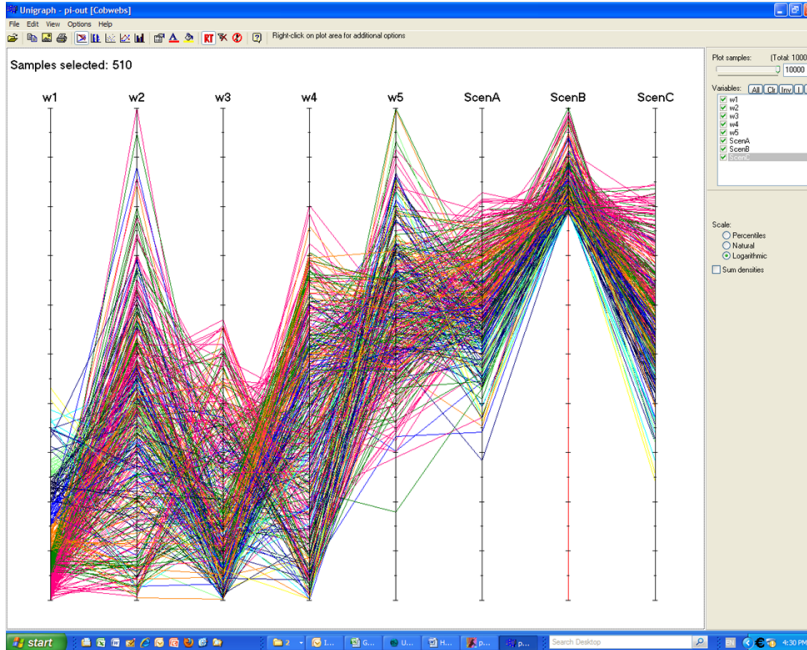


Figure A.2.15: Cob web Plot Joint Distribution



**Figure A.2.16:** Cob web Plot Conditioned on *ScenA* and *ScenB* Relatively Low and Weight  $w_2$  High



## 9. Out-of-sample Validation

Validation of the utility model is achieved by predicting the ranking probabilities from the validation set. In this case the validation is quite decent. The "fitted" columns show the probabilities given by the experts, and those recovered by PI. They are quite close. The "predicted" columns show the same for the first rank probabilities which were NOT used to fit the model. We see that the agreement is somewhat less, but still quite decent. In many applications the agreement is not so close. The Weights table A.2.17 shows that  $w_2$  has a mean value over the stakeholders of 0.16; the others are all around 0.2. All weights except  $w_2$  are about equally important.

Figure A.2.17: Out of sample validation

PREDICTED			FITTED		
	EXPERTS	PI		EXPERTS	PI
A1	0.0645	0.0704	I2	0.0569	0.0564
B1	0.0161	0.0549	K2	0.0569	0.0584
C1	0.0161	0.0322	M2	0.0732	0.0708
D1	0.0403	0.0268	Q2	0.0732	0.0718
E1	0.0484	0.0567	R2	0.0813	0.0843
F1	0.0242	0.0351	S2	0.0894	0.0895
G1	0.0040	0.0224	I3	0.1057	0.1040
H1	0.0040	0.0314	J3	0.0894	0.0904
I1	0.1371	0.0618	M3	0.0325	0.0313
J1	0.1774	0.0660	Q3	0.0569	0.0580
K1	0.0645	0.0456	S3	0.0650	0.0637
L1	0.0081	0.0282	A4	0.0732	0.0726
M1	0.0565	0.0472	E4	0.0569	0.0558
N1	0.0323	0.0686	I4	0.0732	0.0728
O1	0.0484	0.0735	J4	0.0569	0.0535
P1	0.0161	0.0367	K4	0.0813	0.0849
Q1	0.1210	0.0784	M4	0.1057	0.1080
R1	0.0645	0.0829	Q4	0.0569	0.0575
S1	0.0242	0.0354	S4	0.0650	0.0644
T1	0.0323	0.0456	A5	0.0569	0.0567
			E5	0.0732	0.0695
			F5	0.0650	0.0651
			I4	0.0976	0.0976
			J5	0.0650	0.0654
			K5	0.0732	0.0715
			Q5	0.0732	0.0763
			R5	0.0650	0.0651

WEIGHT			
	MEAN	VARIANCE	STDEV
W1	0.2110	0.0129	0.1136
W2	0.1650	0.0110	0.1049
W3	0.2020	0.0124	0.1114
W4	0.2050	0.0131	0.1145
W5	0.2170	0.0134	0.1158

CORRELATION					
	W1	W2	W3	W4	W5
W1	1	-0.27	-0.2	-0.24	-0.29
W2	-0.27	1	-0.19	-0.22	-0.2
W3	-0.2	-0.19	1	-0.29	-0.26
W4	-0.24	-0.22	-0.29	1	-0.23
W5	-0.29	-0.2	-0.26	-0.23	1





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# Summary

## Discrete Decisions with Model Validation using Probabilistic Inversion

Discrete choice denotes the choice behavior of a group of stakeholders. The assumption widely used in discrete choice is that a distribution over utility values of the choices can be inferred from a distribution over preferences of the stakeholders. Despite a wide range of literature on discrete choice and its applications, there is little attention to the validation of the models used in discrete choice. Validation aims to promote transparency and the ability to make predictions based on the decision model.

In this study a mathematical framework is formulated for decisions making using group preferences. This framework formulates decision models based on group preferences as a probabilistic inverse problem. The benefits that result from using this framework are that preferences are better expressed in the decision models, but more importantly, it provides an opportunity for validation.

The first part of the thesis focuses its attention on the assumptions made in discrete choice and introduces the notion of model validation. One of these assumptions is the so called *Independence of Irrelevant Alternatives* paradox that will be covered in chapter 2 of the thesis. In chapter 3 the problem of discrete choice is formulated as a constraint optimization problem. The optimal distribution from this constraint optimization problem is not always independent with respect to the utility values of the choices as often assumed. Further when the number of alternatives increases conventional solution techniques for constraint optimization become intractable, but a approximation of the solution can still be obtained using *Probabilistic Inversion*.

The second part of the thesis applies the theory developed to three case studies and validates the models used in each of the studies. The first application in chapter 4 concerns the budget allocation of ecosystem conservation in the California coastal area[71, 90]. The criteria used in this MCDM model intend to

capture the vulnerability of the ecosystems. Weights fitted to the model are used to determine the threat potential of all the remaining ecosystems.

The second application is given in 5. The idea of modeling health states as a random utility model with underlying physical attributes is not new [81]. Whereas these studies attempt to extract valuations on criteria (criteria weights), this study aimed to improve an existing model EQ-5D+C for valuing health states using stakeholders' preferences on health states directly. The idea is that applying stakeholders preferences to the model will lead to more transparent and defensible assessment of the MCDM model.

The most recent and last application is given in chapter 6. Our techniques for MCDM are applied to find a basic screening model for the safety of nanotechnology enabled food products. Although the benefits of using nano-particles in food products is clear, i.e. fewer quantities needed, the risks have yet to be determined. Doing a case by case study is not possible, because there is few to no data available about the safety of nanotechnology enabled food products. With stakeholders' preferences and probabilistic inversion we capture knowledge about the safety of these products and use the preferences to fit a screening model based on a set on 10 criteria.

Some important results from this research and applications have emerged. First validation is possible for decision models using group preferences, but further research is needed to find the best way of validation. Secondly, there are other forms of decision models possible with the established framework than the often used linear models. And finally, more information can be distilled from the decision models using the established framework of this study.

*Rabin Neslo*



# Samenvatting

## Discrete Beslissingen en Model Validatie met behulp van Stochastische Inverse

Het onderzoeksgebied *discrete choice* houdt zich bezig met de keuzes van belanghebbenden. De aanname die meestal wordt gebruikt in discrete choice is dat er een kansverdeling over the nutswaarden van de keuzen kan worden afgeleid naar aanleiding van een kansverdeling over de preferenties van de belanghebbenden. Ondanks een breed scala aan literatuur betreffende beslismodellen en hun toepassingen, wordt er weinig aandacht besteedt aan het valideren van deze beslismodellen. Validatie heeft als doel het bevorderen van transparantie en de mogelijkheid voorspellingen te kunnen aan de hand van het model.

In dit onderzoek wordt als eerst een wiskundig kader opgesteld voor beslissingen die gebruik maken van groepspreferenties. Dit kader formuleert beslismodellen aan de hand van groepspreferenties als een stochastisch inverse probleem. De voordelen die hieruit volgen bieden de mogelijkheid om preferenties beter tot uiting te brengen in de beslismodellen, maar nog belangrijker : het biedt een mogelijkheid voor validatie.

Het eerste deel van het proefschrift richt zijn aandacht op de aannames op het gebied van discrete keuze en introduceert het concept van validatie. Een van deze aannames is de zogenaamde *Onafhankelijkheid van irrelevante alternatieven* paradox die aan bod komt in hoofdstuk 2 van het proefschrift. In hoofdstuk 3 wordt het probleem van discrete keuze geformuleerd als een optimalisatie probleem. De optimale kansverdeling over de nutswaarden blijkt niet in alle gevallen onafhankelijk zoals meestal wordt verondersteld. Verder volgt ook dat wanneer het aantal keuzen toeneemt conventionele oplossings technieken moeilijk een oplossing kunnen vinden, maar dat een oplossing nog steeds kan worden verkregen met behulp van *Stochastische Inverse*.

In het tweede deel wordt de theorie toegepast in drie studies en valideert de modellen die in elk van de studies worden gebruikt. De eerste toepassing in hoofdstuk 4 betreft de toewijzing van budgetten voor ecosysteem behoud in het Californische kustgebied. De criteria die zijn gebruikt in dit model beoogde de kwetsbaarheden van de ecosystemen vast te leggen. Gewichten voortvloed uit het model worden gebruikt om de kwetsbaarheden van de resterende ecosystemen te bepalen.

De tweede toepassing is gegeven in hoofdstuk 5. Het idee van het modelleren van de gezondheid toestanden als een willekeurige gebruiksmodel met een onderliggende fysieke eigenschappen is niet nieuw. Overwegende worden in dit soort type studies getracht om waarderingen van criteria (criteria gewichten) te bepalen, deze studie richtte zich op het verbeteren van een bestaand model EQ-5D + C. Het idee is dat het toelaten van belanghebbenden hun keuzepatronen in het model zal leiden tot meer transparantie en verdedigbaar de beoordeling van het model.

De meest recente en laatste toepassing wordt gegeven in hoofdstuk 6. Onze technieken voor worden toegepast om een basis screening model voor de veiligheid van nano-gemodificeerde voedingsproducten te vinden. Hoewel de voorordelen van het gebruik van nano-deeltjes in voedingsproducten duidelijk is, bijvoorbeeld het gebruik van minder hoeveelheden, moeten de risico's nog worden bepaald. Het doen van toepassingsgerichte studies is niet mogelijk, omdat er weinig tot geen gegevens beschikbaar zijn over de veiligheid van nano-gemodificeerde voedingsproducten. Met expertise van belanghebbenden en stochastische inverse kunnen we de kennis omtrent de veiligheid van deze producten vastleggen en kunnen de voorkeuren worden gebruikt om een screening model gebaseerd op 10 criteria te bepalen.

Er zijn een aantal belangrijke resultaten uit dit onderzoek en de toepassingen naar voren gekomen. Ten eerste is validatie mogelijk voor beslismodellen die gebruik maken van groep preferenties. Ten tweede zijn er ook andere vormen van beslismodellen mogelijk met het opgezette kader dan de zo vaak gebruikte lineaire modellen. En ten slotte kan meer informatie worden gedestilleerd uit de beslismodellen die gebruik maken van het opgezette kader van dit onderzoek.

*Rabin Neslo*



# Curriculum Vitae

Rabin Neslo was born in Paramaribo on 20 October, 1982. After finishing his high school he moved to The Netherlands to study Applied Mathematics at the Delft University of Technology. He was privileged to finish his study at the Joint Research Center of the European Commission and graduated in 2006. His thesis topic was entitled *A New Participatory Framework to Build and Interpret Composite Indicators: An Application to Country Competitiveness* graduated. The research of his Master Of Science thesis lead to him becoming a PhD student (in Dutch: *Beursaal Assistent in Opleiding* or Beursaal AIO) with the Faculty of Applied Mathematics at the Delft University of Technology (TU Delft). His need to apply his knowledge and his eagerness to explore new things has resulted in him reducing his time at the TU Delft to start at PricewaterHouseCoopers (PwC) in Amsterdam. He held the position for one year as real-estate tax advisor, but due to the financial crisis that hit late 2008 he was forced to discontinue this path and fully pick up his PhD study in Delft.





