

1 A tool to guide the selection of impact categories for
2 LCA studies by using the Representativeness Index

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18 ABSTRACT

19 Understanding the environmental profile of a product computed from the Life Cycle Assessment
20 (LCA) framework is sometimes challenging due to the high number of environmental indicators
21 involved. The objective here, in guiding interpretation of LCA results, is to highlight the
22 importance of each impact category for each product alternative studied. For a given product, the
23 proposed methodology identifies the impact categories that are worth focusing on, relatively to a
24 whole set of products from the same cumulated database.

25 The approach extends the analysis of Representativeness Indices (RI) developed by Esnouf et al.
26 (2018). It proposes a new operational tool for calculating RIs at the level of impact categories for
27 a Life Cycle Inventory (LCI) result. Impact categories and LCI results are defined as vectors within
28 a standardized vector space and a procedure is proposed to treat issues coming from the correlation
29 of impact category vectors belonging to the same Life Cycle Impact Assessment (LCIA) method.
30 From the cumulated ecoinvent database, LCI results of the Chinese and the German electricity
31 mixes illustrate the method. Relevant impact categories of the EU-standardised ILCD method are
32 then identified. RI results from all products of a cumulated LCI database were therefore analysed
33 to assess the main tendencies of the impact categories of the ILCD method. This operational
34 approach can then significantly contribute to the interpretation of the LCA results by pointing to
35 the specificities of the inventories analysed and for identifying the main representative impact
36 categories.

37

38 **KEYWORDS:** LCA, Life Cycle Inventory, Life Cycle Impact Assessment, representativeness,
39 dimension reduction, interpretation tools

40

41 **1. Introduction**

42 While the main goal of the Life Cycle Assessment (LCA) framework is to quantify and assess all
43 the potential environmental impacts of human activities (ISO, 2006), the study of results over a
44 too wide range of environmental impacts can become inefficient and lead to unclear conclusions
45 (Steinmann et al., 2016). To obtain those environmental impact results, the LCA framework is
46 structured in four phases where the Life Cycle Inventory (LCI) phase is one of the key one; it
47 describes a product, a process or an activity throughout its value chain and quantifies its system-
48 wide emissions and resource extractions. An LCI database (of which ecoinvent (Wernet et al.,
49 2016) is a prime example) contains a large number of unit processes, each of which specifies the
50 inputs and outputs (such as electricity, plastic, fossil resources and pollutants) of activities (such
51 as rolling steel or driving a truck). Those LCI unit process databases allow LCA practitioners
52 modelling the whole value chain of their study in reasonable time. The result of an LCI is a list of
53 quantified emissions and resource extractions, collectively indicated as elementary flows,
54 aggregated over all (up to thousands) unit processes that make up the system. In a cumulated LCI
55 database, the entries are not the unit processes but rather the system-wide elementary flows, for
56 each included product. From the LCI result, the Life Cycle Impact Assessment (LCIA) phase then
57 translates these elementary flows in terms of environmental impacts. Different LCIA methods are
58 available, often with a name, such as ReCiPe (Goedkoop et al., 2009), Traci (Bare, 2011) and
59 ILCD (EC-JRC, 2010a). Each LCIA method consists of a number of environmental impact
60 categories (such as global warming and ecotoxicity) and proposes Characterization Factors (CFs)
61 to quantitatively link the elementary flows to these impact categories. There are often ten or more
62 such impact categories within each LCIA method (EC-JRC, 2010b). Although aiming at being

63 holistic, such large sets of impact categories can challenge the efficiency of environmental
64 regulations (like product eco-design, decision making or environmental labelling). Further
65 modelling the impacts into so-called endpoint damage levels could resolve the issue related to
66 large sets. However, due to uncertainties, all models which are presently available are still
67 classified as “interim” (Hauschild et al., 2013).

68 A reduction in the number of impact categories, by selecting the most relevant impact categories
69 to focus on, would enable more effective environmental optimization. For comparative LCA,
70 existing practices for normalization and weighting use external valuation of impact categories that
71 might guide LCA practitioners on a reduced subset of LCIA results to interpret (Lautier et al.,
72 2010). However, these procedures are increasingly discouraged (Prado-Lopez et al., 2014). By
73 quantifying the uncertainties, exploration of the relative importance of impact categories through
74 the magnitude of differences between LCIA results can produce promising tools for comparative
75 LCA (Mendoza Beltran et al., 2018).

76 Some authors used Principal Component Analysis (PCA), combined with uncertainty analysis or
77 multi-objective optimization (Mouron et al., 2006; Pozo et al., 2012) to deal with the large number
78 of environmental indicators. Sometimes, PCA was also applied on LCIA results with technical
79 indicators to reveal the relationships between those indicators (Basson and Petrie, 2007; Bava et
80 al., 2014; Chen et al., 2015; De Saxcé et al., 2014).

81 Steinmann et al. (2016) applied PCA over a large range of products and LCIA methods (all the
82 LCIA results of 135 impact categories for 976 products provided byecoinvent) to select impact
83 categories. In order to deal with impact category units and the wide orders of magnitude of LCIA
84 results due to the high diversity of reference flows, they proposed to apply a product ranking. An

85 alternative approach was a log-transformation on LCIA results prior to using a multi-linear
86 regression (Steinmann et al., 2017). As comment to this last article, Heijungs (2017) noticed that
87 the reference flow values of the studied LCIA results affect the outcomes of their work. He
88 suggested standardizing the LCIA results by their energy footprint to be free of the default
89 reference flow. This emphasizes the need to address data heterogeneity.

90 Other studies that apply multivariate statistical analysis or multi-linear regression on LCIA results
91 of products fromecoinvent focus on revealing correlation or alleged redundancies between impact
92 categories (Huijbregts et al., 2006; Pascual-González et al., 2016, 2015; Steinmann et al., 2017).
93 The objectives of these studies were to predict LCIA results from a reduced number of proxy
94 impact categories. All these approaches work on the impact category results alone, and do not
95 consider LCI information and its translation to impact categories.

96 By translating the elementary flows in terms of impact categories, LCIA can be considered to be
97 a dimension reduction technique: LCIs are described by LCI results with more than a thousand
98 variables (elementary flows) while LCIA results are a much smaller number of environmental
99 indicators. The remaining dimensions, which all have an environmental meaning, may not all be
100 necessary for dealing with the main environmental issues of the studied product. As the
101 environment is disturbed and even damaged by such diverse substance emissions or resource
102 utilizations from different human activities, all impact categories should be covered, but some of
103 them may not be essential for the conclusion of one particular product, for instance, because they
104 are strongly correlated with other impact categories.

105 The Representativeness Index (RI) was recently proposed by Esnouf et al. (2018) to provide a
106 relative measure of the discriminating power of LCIA methods. The RI is meant to explore the

107 relative relevance of each impact category belonging to a LCIA method for a specific product. It
108 does not assess the relevance of the environmental model behind impact categories of the LCIA
109 methods, but it is an aid to LCA practitioners, so they might focus on a reduced number of impact
110 categories that best represent the elementary flows associated with a particular product. Moreover,
111 by studying the links between the RI of an entire LCIA method and the RIs of its constituent impact
112 categories, some issues have been raised on the correlation of the representativeness of impact
113 categories (Esnouf et al. (2018)).

114 The aim of this paper is to further develop the potential benefits of the RI methodology and to
115 discuss representativeness issues regarding non-orthogonal (i.e. dependent) impact categories, and
116 ways to solve such issues. We also developed an operational tool to calculate RIs as a
117 downloadable Python package from an open access deposit.

118 The present paper is organized as follows: in Section 2, the standardization of the vector space
119 where the LCA study takes place and the proximity relationship between an LCI vector and LCIA
120 method subspaces (or impact category vectors) is briefly revisited as it is the same framework as
121 that explained in Esnouf et al. (2018). The algorithm of orthogonalization of impact categories to
122 avoid redundancy issues within a LCIA method is presented. The approach is illustrated and
123 discussed in Section 3 on the ILCD method for two products results from the cumulatedecoinvent
124 database (Wernet et al., 2016). Main tendencies of RI results over the cumulated LCI database are
125 then explored. The main representative dimensions that support most of the RI values are then
126 determined. Finally, results from the decorrelation algorithm are analysed over the entire
127 cumulated LCI database.

128 **2. Material and method**

129 Table 1 lists notations that are used in the present work. Vectors and matrices are distinguished
 130 from scalar by being written in bold, matrices are moreover capitalized.

131 **Table 1.** List of symbols and their meaning

Symbol	Meaning
m	Number of products in LCI database
n	Number of elementary flows
p	Number of impact categories in a LCIA method
\mathbf{g}_i	LCI result vector of the i^{th} product ($i = 1, \dots, m$)
$g_{x,i}$	The amount of the x^{th} elementary flow for the i^{th} product ($i = 1, \dots, m; x = 1, \dots, n$)
\mathbf{q}_j	The vector of characterization factors of the j^{th} impact category: an impact category vector ($j = 1, \dots, p$)
$q_{x,j}$	The characterization factor of the j^{th} impact category for the x^{th} elementary flow ($j = 1, \dots, p; x = 1, \dots, n$)
\mathbf{Q}	LCIA method matrix composed of a set characterization vectors of p impact categories
$h_{j,i}$	LCIA result of the i^{th} product on the j^{th} impact category ($i = 1, \dots, m; j = 1, \dots, p$)
G_x	Geometric mean of $g_{x,i}$ for the x^{th} elementary flow ($x = 1, \dots, n$)
$\tilde{\mathbf{g}}_i$	Standardized form of \mathbf{g}_i (using the geometric mean) ($i = 1, \dots, m$)
$\tilde{\mathbf{q}}_j$	Standardized form of \mathbf{q}_j (using the geometric mean) ($j = 1, \dots, p$)
$\tilde{\mathbf{Q}}$	LCIA method matrix consisting of standardized impact vectors $\tilde{\mathbf{q}}_j$
$\gamma_{j,i}$	Angle between $\tilde{\mathbf{q}}_j$ and $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m; j = 1, \dots, p$)
$\tilde{\mathbf{q}}_j^\perp$	Orthogonalized form of $\tilde{\mathbf{q}}_j$ (from a Gram-Schmidt process) ($j = 1, \dots, p$)
$\tilde{\mathbf{Q}}^\perp$	LCIA method matrix consisting of orthogonalized impact vectors $\tilde{\mathbf{q}}_j^\perp$
$RI_{j,i}$	Representativeness index of $\tilde{\mathbf{q}}_j$ for $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m; j = 1, \dots, p$)
RI_i	Representativeness index of LCI-result $\tilde{\mathbf{g}}_i$ for all impact categories ($i = 1, \dots, m$)
$RI_{j,i}^\perp$	Orthogonal representativeness index of $\tilde{\mathbf{q}}_j^\perp$ for $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m; j = 1, \dots, p$)
RI_i^\perp	Orthogonal representativeness index of LCI-result $\tilde{\mathbf{g}}_i$ for all orthogonalized impact categories ($i = 1, \dots, m$)
$RI_{j,i}^{\text{decorr}}$	Decorrelated representativeness index of $\tilde{\mathbf{q}}_j$ for $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m; j = 1, \dots, p$)
SRR_j	Sum of squared correlation coefficients of $\tilde{\mathbf{q}}_j$ and all other $\tilde{\mathbf{q}}$ -vectors ($j = 1, \dots, p$)
Θ_j	A set of impact category vectors that are correlated to \mathbf{q}_j and belonging to \mathbf{Q} ($j = 1, \dots, p$)
S_i	Sum of squared RIs over $t = 1, \dots, p$ ($i = 1, \dots, m$)
k	Iteration round ($k = 2, \dots, p$)

$R_{t,i,k}$	RI result of the $\tilde{\mathbf{q}}_t$ for $\tilde{\mathbf{g}}_i$ and treated during the iteration k ($t = 1, \dots, p; i = 1, \dots, m; k = 2, \dots, p$)
$d_{j,i}$	Distance between $RI_{j,i}$ and $RI_{j,i}^\perp$ ($i = 1, \dots, m; j = 1, \dots, p$)
$\langle \mathbf{x}, \mathbf{y} \rangle$	Inner product of vectors \mathbf{x} and \mathbf{y}
$\ \mathbf{x}\ $	Norm (Euclidean length) of vector \mathbf{x}

132

133 2.1. RI methodology

134 2.1.1. Standardization and definition of an inner product

135 As proposed by several authors (Esnouf et al., 2018; Heijungs and Suh, 2002; Téo, 1999) the
 136 vector space where the LCA framework takes place is generated by a basis that represents the n
 137 elementary flows that are included in the study. The result of the LCI phase, for the i^{th} product,
 138 can be described as a vector \mathbf{g}_i (see Figure 1. **Erreur ! Source du renvoi introuvable.**a.).
 139 However, each component x of such an LCI result vector, so the elementary flows $g_{x,i}$ that form
 140 \mathbf{g}_i , has its own accounting unit (e.g. kilogram, Becquerel, joule...), and within this vector space,
 141 no consistent inner product (which induces a norm) can be defined (Heijungs and Suh, 2002). In
 142 this perspective, it is useful to recall that the vector spaces that are usually employed in the
 143 engineering disciplines refer to 3-dimensional Euclidean space, in which vectors have a magnitude
 144 and a direction, and concepts such as angle and distance make sense. In non-metric vector spaces,
 145 vectors are more abstractly considered to be n -tuples, for which such concepts are not defined
 146 (Gentle, 2007). In order to be able to measure distances or angles between vectors, we here extend
 147 the studied vector space with an inner product after a standardization step.

148 Among the diversity of possible standardizations (min-max, z-score...), the geometric mean of
 149 each elementary flow over all products is used in the present work for two reasons. First, the

150 geometric mean is robust to extreme values. Secondly and more importantly, this choice allows
 151 our approach being free of the reference flow values of LCI results (i.e. the issue emphasised by
 152 Heijungs (2017) about Steinmann et al. (2017) approach; see the section 2.1.2. and SI A.1 for
 153 details). Defining G_x as the geometric mean of the x^{th} elementary flow, so

$$G_x = \exp\left(\frac{1}{m} \sum_{i=1}^m \ln|g_{x,i}|\right) \quad (1)$$

154 the x^{th} standardized elementary flows $\tilde{\mathbf{g}}_{x,i}$ of the i^{th} LCI result is:

$$\tilde{g}_{x,i} = \frac{g_{x,i}}{G_x} \quad (2)$$

155 Note that we used the absolute value in equation 1 to allow for cases where the values are negative.

156 Within this standardized vector space and given two LCI result vectors $\tilde{\mathbf{g}}_1$ and $\tilde{\mathbf{g}}_2$, we can define
 157 the inner product of these vectors as:

$$\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle = \sum_{x=1}^n \tilde{g}_{x,1} \tilde{g}_{x,2} \quad (3)$$

158 Next, we define the norm or Euclidean length of a vector $\tilde{\mathbf{g}}_i$ as

$$\|\tilde{\mathbf{g}}_i\| = \sqrt{\langle \tilde{\mathbf{g}}_i, \tilde{\mathbf{g}}_i \rangle} \quad (4)$$

159 Finally, this allows us to define the angle α between two LCI vectors, say, $\tilde{\mathbf{g}}_1$ and $\tilde{\mathbf{g}}_2$, indicated by
 160 $\alpha_{1,2}$, as

$$\alpha_{1,2} = \arccos\left(\frac{\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle}{\|\tilde{\mathbf{g}}_1\| \|\tilde{\mathbf{g}}_2\|}\right) \quad (5)$$

161 Within the standardized vector space, the LCI result of each product has then its own vector
 162 direction and norm (see Figure 1.a.).

163 The norm of a standardized LCI result vector still depends on the magnitude of the reference flow
164 of the product, while the direction of the vector doesn't. This justifies the proposed definition based
165 on the angle between vectors (see part 2.1.2).

166 Regarding impact categories, the consequences of unit amounts of the different elementary flows
167 are summarised by their characterization factors (CFs), the numbers $q_{x,j}$. CFs are conversion
168 factors used to assess the elementary flows in terms of impact category results. The collection of
169 CFs of one impact category therefore defines a vector within the elementary flow vector space
170 (according to the Fréchet-Riesz theorem, see Esnouf et al. (2018) section 2.1.2). Figure 1.a.
171 illustrates this for two impact categories, where the vector of CFs is denoted as $\tilde{\mathbf{q}}_1$ and $\tilde{\mathbf{q}}_2$, after
172 standardization (see below).

173 Because we work with standardized elementary flows, the CFs should be standardized as well to
174 maintain unit consistency:

$$\tilde{q}_{x,j} = q_{x,j} G_x \quad (6)$$

175 In this way, by standardizing the impact categories, we can depict the vectors $\tilde{\mathbf{q}}_j$ into the same
176 standardized vector space. It reveals the main dimensions that contribute to each of the modelled
177 environmental issues.

178 The LCIA step of the LCA framework translates the LCI result \mathbf{g}_i into a quantified LCIA result
179 $h_{j,i}$. The scalar $h_{j,i}$ is the amount of impacts on the j^{th} impact category for the i^{th} product using a
180 linear transformation:

$$h_{j,i} = \sum_{x=1}^n q_{x,j} g_{x,i} \quad (7)$$

181 The LCIA result of a standardized LCI result vector $\tilde{\mathbf{g}}_i$ with a standardized impact category $\tilde{\mathbf{q}}_j$
 182 equals to the previous LCIA result $h_{j,i}$ of the unstandardized vectors:

$$\tilde{h}_{j,i} = \langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \rangle = \sum_{x=1}^n q_{x,j} G_x \frac{g_{x,i}}{G_x} = h_{j,i} \quad (8)$$

183 We extend the definition of the inner product of two standardized LCI vectors, say, $\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle$ to the
 184 inner product of two standardized impact categories, say, $\langle \tilde{\mathbf{q}}_1, \tilde{\mathbf{q}}_2 \rangle$, and to the inner product of a
 185 standardized LCI vector and a standardized impact category $\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \rangle$ (previously used in equation
 186 8 for the definition of the LCIA result $\tilde{h}_{j,i}$). This also allows us to define the norm of an impact
 187 category, $\|\tilde{\mathbf{q}}_j\|$, the angle between two impact categories, β , and the angle ($\gamma_{j,i}$) between an LCI
 188 vector $\tilde{\mathbf{g}}_i$ and an impact category vector, $\tilde{\mathbf{q}}_j$. This finally allows us to define the representativeness
 189 index RI between an LCI vector and an impact category, as discussed in the next section.

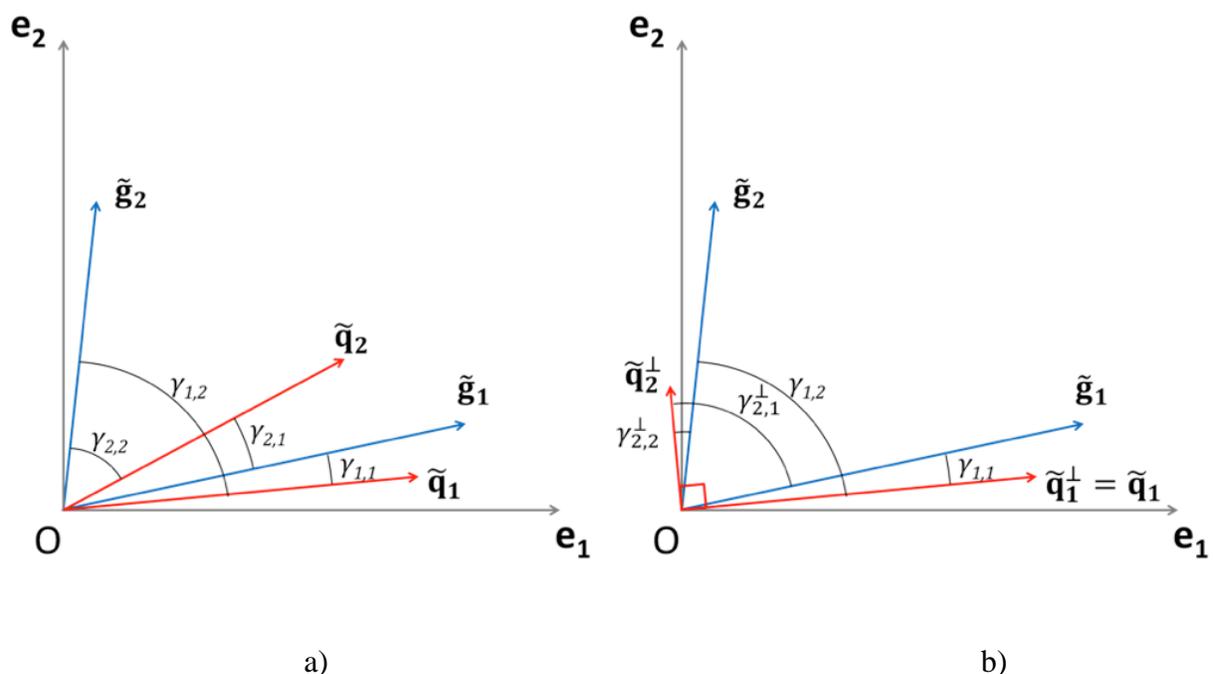
190 2.1.2. RI between a LCI result and an impact category

191 Within a standardized vector space, the representativeness index (RI) proposed by Esnouf et al.
 192 (2018) is a measure between a standardized LCI result ($\tilde{\mathbf{g}}_i$) vector and an impact category vector
 193 ($\tilde{\mathbf{q}}_j$). In order to be free of the norm of the different vectors, it is based on the angle $\gamma_{j,i}$ between
 194 an LCI result vector and an impact category vector. The RI of an LCI result $\tilde{\mathbf{g}}_i$ for the impact
 195 category $\tilde{\mathbf{q}}_j$ is:

$$RI_{j,i} = RI(\tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i) = |\cos(\gamma_{j,i})| = \frac{|\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \rangle|}{\|\tilde{\mathbf{q}}_j\| \|\tilde{\mathbf{g}}_i\|} = \frac{|h_{j,i}|}{\|\tilde{\mathbf{q}}_j\| \|\tilde{\mathbf{g}}_i\|} \quad (9)$$

196 The higher the values of the RI, the better the impact category represents the main dimensions of
 197 the LCI result vector (i.e. the direction), relatively to the cumulated LCI database. Within the

198 standardized vector space, the representativeness index can then be interpreted as a measure of
 199 similarity between the standardized LCI result vector and the standardized impact category vector.



200
 201
 202 **Figure 1.** a) Representation of two standardized LCI result vectors $\tilde{\mathbf{g}}_1$ and $\tilde{\mathbf{g}}_2$ (in blue), two
 203 standardized impact category vectors $\tilde{\mathbf{q}}_1$ and $\tilde{\mathbf{q}}_2$ (in red), and the four of the angles $\gamma_{j,i}$ used to
 204 measure RIs. The vector space is spanned by two basis vectors (\mathbf{e}_1 and \mathbf{e}_2) representing
 205 standardized elementary flows, such as CO₂ and NO_x. b) Illustration of the correlation issue and
 206 $\tilde{\mathbf{q}}_2^\perp$, the orthogonal version of $\tilde{\mathbf{q}}_2$ (see below).

207 2.1.3. RI between a LCI result and a LCIA method

208 In addition to the RI between an LCI result and an impact category, we define the RI between an
 209 LCI result and an entire LCIA method consisting of a collection of impact categories. An LCIA
 210 method can be regarded as a sub-space of the standardized vector generated by the impact

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211 categories. The LCIA method is written as a matrix \mathbf{Q} , consisting of the p different impact
212 categories that belong to that method:

$$\mathbf{Q} = (\mathbf{q}_1 \quad \cdots \quad \mathbf{q}_p) \quad (10)$$

213 Because we decided to work in standardized space, we effectively work with

$$\tilde{\mathbf{Q}} = (\tilde{\mathbf{q}}_1 \quad \cdots \quad \tilde{\mathbf{q}}_p) \quad (11)$$

214 The RI of the entire LCIA method is then defined, for LCI result \mathbf{g}_i , as

$$RI_i = RI(\tilde{\mathbf{Q}}, \tilde{\mathbf{g}}_i) = \sqrt{\sum_{j=1}^p (RI(\tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i))^2} \quad (12)$$

215 2.1.4 Correlation and decorrelation

216 The impact category vectors of the LCIA method are in general not orthogonal, that is, the angle
217 β between some of the (standardized) impact category vectors is not 90 degrees. This also implies
218 that for an LCIA method, subsets of non-orthogonal impact category vectors can be observed for
219 which the impact category vectors are correlated with each other. The effect of this is an over- or
220 under-representation of the LCI result vector by those impact category vectors. It relies on the fact
221 that RIs of the non-orthogonal impact category vectors for the LCI result vector will assess and
222 represent the LCI result vector through the same main elementary flows. Indeed, the main direction
223 of a LCI result vector can be close to the main direction of two (or more) non-orthogonal impact
224 category vectors, which lead to an over-representation, or at the opposite, both impact category
225 vectors miss this main direction even if their characterization factors are not null on the main
226 dimensions of the LCI result vector, which then lead to an under-representation. At the LCIA

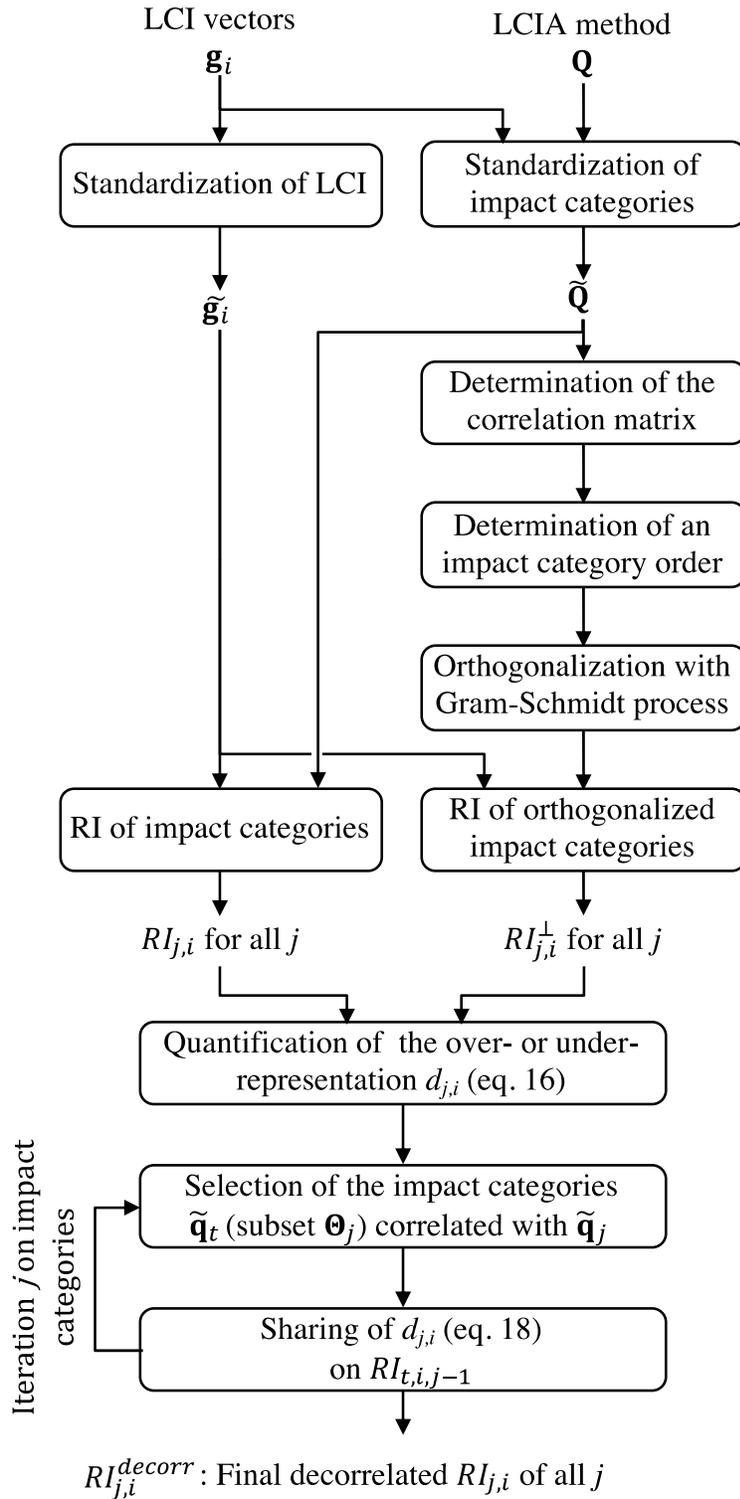
227 method level, this over or under-representation can be solved by an orthogonalization procedure
 228 of the impact category vectors $\tilde{\mathbf{q}}_j$ (Esnouf et al., 2018). This procedure is based on the well-known
 229 Gram-Schmidt process (Arfken and Weber, 2012). The Gram-Schmidt process returns a new set
 230 of standardized perpendicular vectors, which will be denoted here as $\tilde{\mathbf{q}}_j^\perp$ (see Figure 1.b.). Similar
 231 to equation 11, we can pack these vectors for the entire LCIA method in one matrix, $\tilde{\mathbf{Q}}^\perp$. Using
 232 the angle $\gamma_{j,i}^\perp$ between an LCI result vector $\tilde{\mathbf{g}}_i$ and an orthogonalized impact category vector $\tilde{\mathbf{q}}_j^\perp$,
 233 this in turn can serve to calculate a new RI of a LCIA method, similar to equations 9 and 12:

$$RI_{j,i}^\perp = RI(\tilde{\mathbf{q}}_j^\perp, \tilde{\mathbf{g}}_i) = |\cos(\gamma_{j,i}^\perp)| \quad (13)$$

234 and

$$RI_i^\perp = RI(\tilde{\mathbf{Q}}^\perp, \tilde{\mathbf{g}}_i) = \sqrt{\sum_{j=1}^p (RI_{j,i}^\perp)^2} \quad (14)$$

235 The procedure that is proposed to take into account the over or under-representation for the RIs of
 236 impact category belonging to the same LCIA method is schematized in Figure 2. The upper part
 237 describes the steps that are needed to obtain RI_i and RI_i^\perp that are needed to take out the
 238 consequences of the correlations between impact category vectors. The lower part describes the
 239 iterative loop developed in section 2.1.5. that is needed to solve the consequences triggered by the
 240 order dependency of the impact category that is inherent in the Gram-Schmidt process.



241

242 **Figure 2.** Schematics of the proposed algorithm

243 The Gram-Schmidt process allows obtaining a set of orthogonal impact category vectors from one
 244 LCIA method and thus allows determining its RI_i^\perp . But the order of processing the different $\tilde{\mathbf{q}}_j$
 245 vectors in $\tilde{\mathbf{Q}}$ determines the RIs of the standardized and orthogonalized vectors. With the Gram-
 246 Schmidt iterative process, the first treated vector is not modified (and its RIs will not be different
 247 between $\tilde{\mathbf{q}}_1$ and $\tilde{\mathbf{q}}_1^\perp$) while the next vectors are orthogonalized paying regard to the previously
 248 handled vectors (and there will be differences between the RIs of $\tilde{\mathbf{q}}_j$ and $\tilde{\mathbf{q}}_j^\perp$ (for $j = 2, \dots, p$)).
 249 Because of that, the orthogonalized impact category vectors that result from the Gram-Schmidt
 250 process cannot be directly used to look at the RIs of $\tilde{\mathbf{g}}_i$ for uncorrelated impacts due to this order
 251 dependency.

252 To solve the problem of order-dependency we define a unique order of treatment of the impact
 253 categories. Instead of applying Gram-Schmidt to the usual order $j = 1, \dots, p$, we first sort the
 254 impact category vectors, and apply the Gram-Schmidt process to the vectors arranged in that new
 255 order. This order is determined by using the correlation matrix of the impact category vectors
 256 belonging to $\tilde{\mathbf{Q}}$ (see Figure 2). This makes sense because the correlation coefficient of two vectors
 257 is equivalent to the cosine of the angle between these vectors (Gniazdowski, 2013), which in turn
 258 is equal to the RI as defined above. For each impact category, the sum of the squares of all its
 259 correlation coefficients (SSR) is calculated:

$$SSR_j = \sum_{l=1}^p \left(r(\tilde{\mathbf{q}}_j, \tilde{\mathbf{q}}_l) \right)^2 \quad (15)$$

260 This includes the trivial case $l = j$, for which $r = 1$, but because it doesn't affect the ranking we
 261 can leave it in. The order of impact categories is determined by ranking these sums SSR_j in

262 descending order. The first impact category to be processed is then the one which has the highest
 263 *SSR*, and the maximal correlation with the other impact categories.

264 The over- or under-representation of an LCI result vector by a set of impact category vectors
 265 corresponds to the difference between the RIs measured by the non-orthogonal impact categories
 266 and the RIs measured by the orthogonalized impact categories. Based on the determination of those
 267 differences, a decorrelation algorithm is proposed in the next section. This algorithm allows
 268 distributing the over- or under-representation between the non-orthogonal impact categories
 269 (iteration loop in Figure 2).

270 2.1.5. Decorrelation algorithm of impact category RIs

271 From the $RI_{j,i}^\perp$ determined for a LCIA method after the Gram-Schmidt process, the over- or under-
 272 representation need to be quantified and distributed over the subset of non-orthogonal impact
 273 categories. For the LCI vector $\tilde{\mathbf{g}}_i$ and the impact category $\tilde{\mathbf{q}}_j$, the RI of the orthogonalized impacts
 274 ($RI_{j,i}^\perp$) is compared to the original one ($RI_{j,i}$). Their distance $d_{j,i}$ (as defined in equation 14) is
 275 interpreted as the over- or under-representation of $\tilde{\mathbf{g}}_i$ expressed by the impact category j and that
 276 is redundant or missing regarding the categories that have been previously processed given the
 277 order of the impact categories used in the Gram-Schmidt process:

$$d_{j,i} = \sqrt{(RI_{j,i})^2 - (RI_{j,i}^\perp)^2} \quad (16)$$

278 The over- or under-representation $d_{j,i}$ of the impact category $\tilde{\mathbf{q}}_j$ has to be distributed over the other
 279 non-orthogonal impact categories. For this purpose, each $d_{j,i}$ is treated iteratively with the same
 280 order that is used for impact categories in the Gram-Schmidt process. Let Θ_j be the subset of the

281 category vectors $\tilde{\mathbf{q}}_t$ that are correlated to $\tilde{\mathbf{q}}_j$, $\Theta_j = \{\tilde{\mathbf{q}}_t | t \in \{1, \dots, p\}, r(\tilde{\mathbf{q}}_t, \tilde{\mathbf{q}}_j) \neq 0\}$. $RI_{t,i,j}$ is the
 282 RIs modified by the decorrelation process of the LCI result vector $\tilde{\mathbf{g}}_i$ for the impact category $\tilde{\mathbf{q}}_t$
 283 during the j^{th} iteration. For the first impact category treated $d_{1,i} = 0$ ($RI_{1,i}^\perp$ is equal to $RI_{1,i}$ because
 284 $\tilde{\mathbf{q}}_1$ is not modified by the Gram-Schmidt process, so $\tilde{\mathbf{q}}_1^\perp = \tilde{\mathbf{q}}_1$). Consequently, the results $RI_{t,i,1}$ of
 285 $\tilde{\mathbf{g}}_i$ for these categories $\tilde{\mathbf{q}}_t$ are the original RIs that are obtained from equation 9:

$$RI_{t,i,1} = RI_{t,i} \quad (17)$$

286 Let $S_i = \sum_{t=1}^p (RI_{t,i,1})^2$ the sum of the squares of $RI_{t,i,1}$. For the following iterations ($j = 2, \dots, p$),
 287 all the $RI_{t,i,j}$ will share the over or under-representation measured by $d_{j,i}$:

$$RI_{t,i,j} = \sqrt{(RI_{t,i,j-1})^2 - (d_{j,i})^2 \times \frac{(RI_{t,i,1})^2}{S_i}} \quad (18)$$

288 At the end of the iteration procedure, all the resulting decorrelated RIs, $RI_{j,i}^{\text{decorr}} = RI_{t,i,p}$, of $\tilde{\mathbf{g}}_i$
 289 for the impact category vectors of an LCIA method obtained through this algorithm are free from
 290 the consequences of the order of the impact category used within the Gram-Schmidt process.

291 2.2. Material

292 The methodology is applied to the cumulated LCI result version of the ecoinvent 3.1 “allocation
 293 at the point of substitution” database (Wernet et al., 2016). This version of the cumulated LCI
 294 database was released in 2014. It comprises 11,206 LCI result vectors that are described through
 295 1,727 elementary flows (the intervention matrix). The elementary flows vector space therefore has
 296 1,727 dimensions. Compared to Esnouf et al. (2018), the same matrix was used although certain
 297 elementary flows and LCI results were removed from the cumulated LCI database. Indeed,
 298 considering that the analysis is applied to LCI results, the 70 LCI results that have only less than

299 30 referenced elementary flows are set aside. 142 elementary flows were also not taken into
300 account due to the low number of LCI results that take value on them.

301 The ILCD V1.05 (EC-JRC, 2010a) is the studied LCIA method. It was extracted from the SimaPro
302 8.1.1.16 software to analyse the most recent and operational version. The CF nomenclature was
303 transferred from the SimaPro nomenclature to the ecoinvent elementary flows nomenclature with
304 the assistance of the ecoinvent centre.

305 Implementation was conducted with Python 2.7 on a Jupyter Note-book (Perez and Granger, 2007)
306 (formerly IPython Notebook) and using numerical computation libraries SciPy (V 0.16.0), Pandas
307 (V 0.17.1) and Matplotlib (V 1.5.0). Python is an open-source programming language which is
308 increasingly used in data sciences and in LCA framework as in Brightway2 (Mutel, 2017).

309 An operational tool written with Python 3.6 was also developed. It is available from an online
310 deposit hosted on github.com with the DOI: 10.5281/zenodo.1068914. The package allows to
311 apply the methodology on LCI result excel files (system process) exported from SimaPro and
312 modelled within the ecoinvent 3.1 “allocation at the point of substitution” database (further
313 development needs to be done to apply the methodology to other cumulated LCI databases and to
314 cumulated LCI result files exported from other software). Three outputs can be obtained per LCI
315 result: RIs of LCIA methods, RIs of their impact category vectors and RIs of decorrelated
316 categories. Almost all the multi-criteria LCIA methods can be analysed. Standardization is applied
317 with geometric means of elementary flows after a nomenclature translation from ecoinvent to
318 SimaPro.

319 Based on the studied cumulated LCI ecoinvent database, the LCI results of the Chinese and the
320 German electricity production mixes serve as an illustrative example of the presented work. The

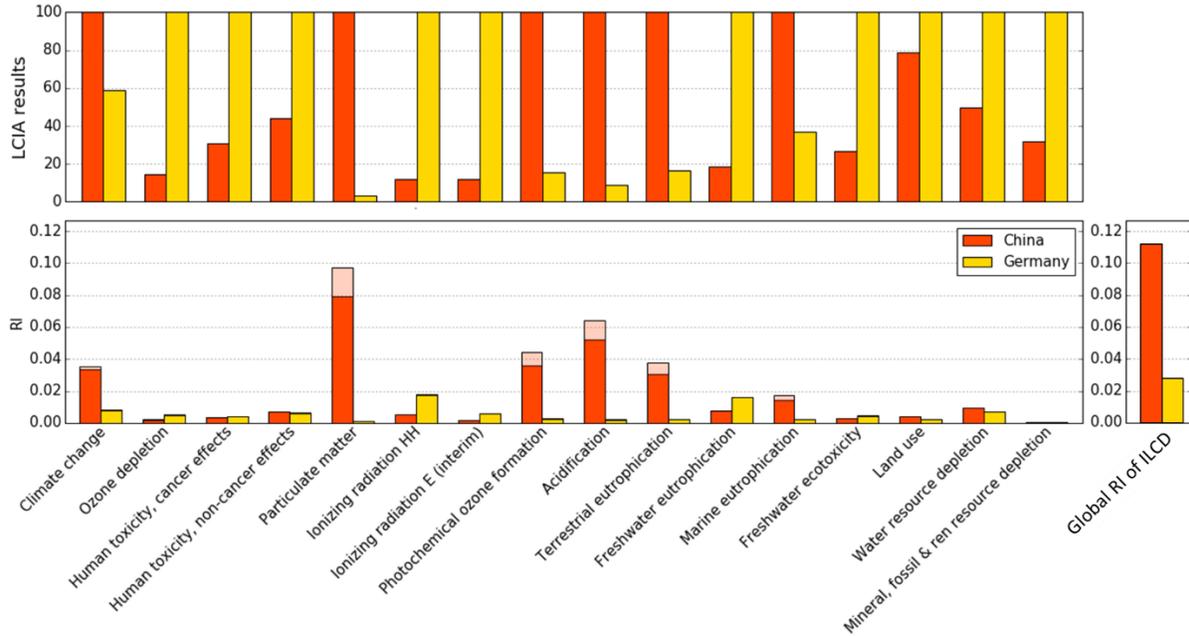
321 two LCI results refer to the market production of 1 kWh of high voltage electricity. The market
322 version of these LCI results models the elementary flows of electricity production mixes,
323 transmission networks and electricity losses during transmission.

324 **3. Results and discussion**

325 **3.1. Illustrative example**

326 3.1.1. LCIA results analysis with respect to RIs

327 A comparison of LCIA results from the Chinese and the German electricity mixes points to a
328 number of noteworthy elements evidenced by the impact categories RI results (see Figure 3). The
329 upper bar-chart typically illustrates the results of a comparative LCA study, the lower chart
330 represents the outputs of the python package (see data in SI B). For the German mix, ten impact
331 category results are higher than for the Chinese mix, out of the sixteen impact categories of the
332 ILCD method. Germany is two-fold higher for 9 categories: Ozone depletion, Toxicities (cancer
333 and non-cancer effects), Ionizing radiations (human health and ecosystems), Freshwater
334 eutrophication, Ecotoxicity and both Resource depletions. The German mix also uses a higher
335 proportion of land area, but the gap is smaller (China is only 21% lower than Germany on this
336 impact category). Contrasting LCIA results are observed for particulate matter, photochemical
337 ozone formation, acidification and terrestrial eutrophication where China is five times higher than
338 Germany. The same observation can be made for climate change and marine eutrophication but
339 with a lower difference (compared to China, German impacts are lower by 41% and 63%
340 respectively).



341
 342 **Figure 3.** LCIA results (expressed relative to the highest value) and impact category RIs for the
 343 LCI results of the Chinese and German electricity mixes from the ILCD method. Bright colours
 344 correspond to decorrelated RIs $RI_{j,i}^{decorr}$ while pastels colours indicate the part removed from the
 345 original RIs by the decorrelation procedure, $d_{j,i}$.

346 The global RIs of the ILCD method are 0.113 for the Chinese and 0.0285 for the German mix. The
 347 Chinese mix has a better overall representation with this LCIA method because its RI of method
 348 is higher. Using impact category RIs from Figure 3, this high overall RI of the method comes from
 349 high impact category RI results on particulate matter, acidification, photochemical ozone
 350 formation, climate change and terrestrial eutrophication (in decreasing order of contribution).
 351 During interpretation, the focus must, in priority, be put on this reduced set of impact category
 352 vectors.

353 The main representative impact categories for the German mix are ionizing radiation (HH),
354 freshwater eutrophication, climate change, water resource depletion and human toxicity (non-
355 cancer effect). The RIs of these LCIA results are two to three times higher for these impact
356 categories (see Figure 3) and they should be looked at first and foremost for the result
357 interpretation.

358 The environmental issues highlighted for this comparative LCA study are not the same for both
359 LCI results. Given the contextualization of LCI results and impact categories from the cumulated
360 LCI database, the use of $RI_{j,i}$ and $RI_{j,i}^{\perp}$ guides the LCA practitioner in the interpretation of the main
361 representative impact categories for each LCI result.

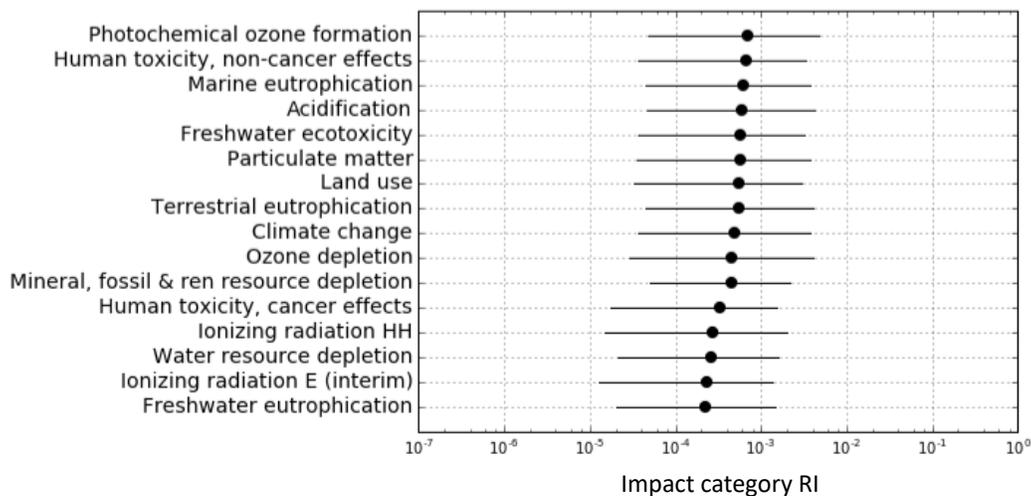
362 3.1.2. Example of decorrelation on two LCI results

363 Results from the decorrelation of impact category RI results obtained for the two previously
364 studied LCI results are presented in the Figure 3. Using the $RI_{j,i}$, the equation 12 results in 0.137
365 and 0.0293, respectively for the Chinese and the German mixes, while the overall RIs of the ILCD
366 method are 0.113 and 0.0285 (see above). These differences a dependence between the impact
367 category vectors, which are removed by the presented algorithm.

368 Six impact category RIs are particularly affected by decorrelation (see Figure 3). The algorithm
369 lowers the representativeness index of the Chinese mix for the particulate matter, acidification,
370 photochemical ozone formation, and terrestrial eutrophication categories. The climate change and
371 marine eutrophication categories are affected to a lesser extent. The decorrelation of the German
372 mix RIs does not affect its representativeness index on any particular impact category.
373 Orthogonalized results do not modify the previous interpretations.

374 **3.2. Global trends of impact category RIs over the cumulated LCI database**

375 The ordered distribution of the impact category RIs of the entire cumulated LCI database indicates
376 that their values rapidly decrease below 0.1, reaching 10^{-2} to 10^{-5} (see Figure 4). These low values
377 result from the high-dimensional vector space in which the study takes place. The ranges of impact
378 category RI values are globally similar when the different impact categories are compared. In an
379 analogous manner, these impact categories represent the different LCI results of the cumulated
380 database, in terms of quantity of information. They all seem relevant for a large number of LCI
381 results. However, all impact categories are probably not compulsory for the analysis of a single
382 LCI result, as observed in the previous illustrative example.



383

384 **Figure 4.** Range of RI values of the ILCD impact categories regarding the 11206 LCI results of
385 ecoinvent. Shown are: the median (dot), the first quartile (left end of line) and third quartile (right
386 end of line). Impact categories are sorted according to their median.

387 **3.3. Decorrelation of impact category RIs within a LCIA method**

388 3.3.1. Correlation matrix of impact categories

389 Table 2 presents the correlation matrix of the impact categories (after standardization). Based on
 390 their correlation, five different subsets of intercorrelated categories (i.e. Θ_j) are labelled from A to
 391 E and described in Table 3. Some impact categories feature in two subsets.

392 **Table 2.** Correlation matrix of impact categories of the ILCD method, on the basis of 11206
 393 products from ecoinvent.

	FWET	HTC	HTNC	ODP	CCP	MEP	TEP	AP	PMP	POFP	IRE	IRHH	MFRDP	WRDP	LU	FWEP
FWET	1	5.3e-1	9.5e-2	2.9e-11	1.4e-13	0	0	0	0	4.0e-9	0	0	0	0	0	0
HTC	5.3e-1	1	1.0e-2	2.0e-7	6.0e-11	0	0	0	0	1.4e-8	0	0	0	0	0	0
HTNC	9.5e-2	1.0e-2	1	1.4e-7	2.9e-11	0	0	0	0	2.6e-7	0	0	0	0	0	0
ODP	2.9E-11	2.0e-7	1.4e-7	1	9.1e-5	0	0	0	0	6.2e-11	0	0	0	0	0	0
CCP	1.4e-13	6.0e-11	2.9e-11	9.1e-5	1	0	0	0	0	1.2e-3	0	0	0	0	0	0
MEP	0	0	0	0	0	1	4.4e-1	1.5e-1	1.2e-2	4.3e-1	0	0	0	0	0	0
TEP	0	0	0	0	0	4.4e-1	1	3.4e-1	2.7e-2	9.7e-1	0	0	0	0	0	0
AP	0	0	0	0	0	1.5e-1	3.5e-1	1	3.3e-1	4.5e-1	0	0	0	0	0	0
PMP	0	0	0	0	0	1.2e-2	2.7e-2	3.3e-1	1	6.7e-2	0	0	0	0	0	0
POFP	4.0e-9	1.4e-8	2.6e-7	6.2e-11	1.2e-3	4.3e-1	9.7e-1	4.5e-1	6.7e-2	1	0	0	0	0	0	0
IRE	0	0	0	0	0	0	0	0	0	0	1	5.7e-1	0	0	0	0
IRHH	0	0	0	0	0	0	0	0	0	0	5.7e-1	1	0	0	0	0
MFRDP	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
WRDP	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
LU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
FWEP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

394

395 **Table 3.** Definition of subsets of impact categories and their abbreviations.

Impact category	Abbreviation	Member of subset				
		A	B	C	D	E
Freshwater ecotoxicity	FWET	X		X		
Human toxicity, cancer effects	HTC	X		X		
Human toxicity, non-cancer effects	HTNC	X		X		
Ozone depletion	ODP	X		X		
Climate change	CCP	X		X		
Marine eutrophication	MEP		X	X		
Terrestrial eutrophication	TEP		X	X		
Acidification	AP		X	X		
Particulate matter	PMP		X	X		
Photochemical ozone formation	POFP	X	X	X		
IRE Ionizing radiation E (interim)	IRE				X	
Ionizing radiation HH	IRHH				X	
Mineral, fossil & renewable resource depletion	MFRDP					X
Water resource depletion	WRDP					X
Land use	LU					X
Freshwater eutrophication	FWEP					X

396

397 The Photochemical ozone formation (within subset C) has a particular position because it
398 correlates with the two subsets A and B which do not have any elementary flows in common. This
399 category is the one with the highest *SSR* (eq. 15) and is therefore the first one to be processed by
400 the algorithm. Consequently, the orthogonalization of one subset A or B does not affect the
401 orthogonalized RI of the other subsets through Photochemical ozone formation relationships.
402 However, the Photochemical ozone formation is affected by both subset A and B.

403 The two ionizing radiation impact categories (subset D) are only correlated with each other. Impact
404 categories that do not correlate with any other are gathered in subset E.

405 The correlation coefficients point out that subsets B and D present very high correlations (between
406 1.17×10^{-2} and 4.44×10^{-1}) in comparison to subset A (from 1.40×10^{-13} to 5.32×10^{-1}).

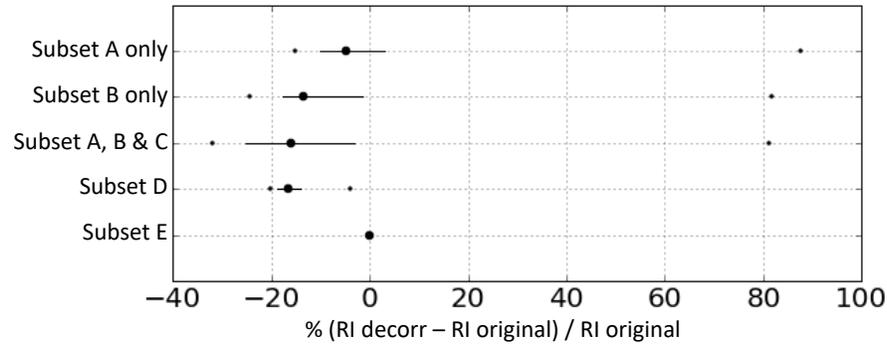
407 The Photochemical ozone formation potential also presents higher correlation coefficients with
408 subset B (up to 9.66×10^{-1}) than with subset A (up to 1.24×10^{-3}).

409 3.3.2. Consequences of decorrelation over the cumulated LCI database

410 Orthogonalized impact category RI values are obtained by applying the algorithm to all 11206
411 ecoinvent LCI results. To determine the global trends of the redistribution of the representativeness
412 of impact categories for all LCI results, the distribution of the ratio $\frac{RI^{decorr}-RI}{RI}$ are analysed for
413 each impact category; see Figure 5. Distributions of the ratio are based on the original RI values
414 and the orthogonalized RI values of the impact categories (see equations 16 and 18). For one LCI
415 result, all the RIs of the impacts categories with a similar belonging to the subsets obtain the same
416 ratio (while each LCI result is associated to a unique ratio). That means with the ILCD method
417 that five group are done: Impact categories only in subset A, only in subset B, in A, B and C (i.e.
418 the Photochemical ozone formation category), in D and in E.

419

420



421

422 **Figure 5.** Analyses of the different redistribution of RI values. Ordinate refers to the belonging of
423 the impact categories. Shown are: the median (large dot), the first quartile (left end of line), the
424 third quartile (right end of line), and the 5% and 95% percentiles (small dots).

425 Results imply that the major part of the redistribution slightly decreases the RI values from $RI_{j,i}$ to
426 $RI_{j,i}^{\text{decorr}}$ (between 0 and 20%). Obviously, impact categories that do not correlate with any other
427 impact category do not show any change (subset E).

428 For subsets A, B and C, a decrease is the main tendency but high increases are observed for some
429 inventories, with a 95% percentiles up to 80% (reaching 300% for extreme values). High values
430 are correlated between the impact categories of these 3 subsets (see SI.A.2). However, for the
431 major part of the impact category RIs (negative modifications down to -20%), the correlation
432 appears to be less obvious. Nevertheless, the modifications remain low for each subset. The wide
433 RI redistribution of the photochemical ozone formation (first impact category treated by the
434 algorithm) is triggered by the orthogonalization from the other two subsets that form another
435 “profile” on Figure 5.

436 As for subset D, the distribution of the modifications in impact category RI is very restricted. This
437 could be explained by the fact that only two impact categories belong to this subset. No correlation
438 of the redistribution with the other subsets is observed (see SI A.2).

439 The increase of RI values for $RI_{j,i}^{\text{decorr}}$ is triggered by the high $RI_{j,i}^{\perp}$ which is observed for several
440 subsets. A LCI result with an high value on an elementary flow, which is not associated to a high
441 CF of any impact categories, can be highlighted by the orthogonalization step and thus lead to an
442 increase in the RI value. The orthogonalization of the impact category redirects the vector towards
443 a secondary elementary flow (see Figure 1.b). When LCI results have a high value on this second
444 elementary flow, their $RI_{j,i}^{\perp}$ tend to increase compared to $RI_{j,i}$. Most of the LCI results characterized
445 by higher $RI_{j,i}^{\perp}$ originate from agricultural production. This is mainly related to ammonia and nitrate
446 elementary flows. The redistribution of extra information from the secondary elementary flow
447 should provide the impact categories of the subset with an increase that finally allows their
448 $RI_{j,i}^{\text{decorr}}$ to comply with the RI of the LCIA method.

449 **4. Conclusions**

450 This work completes the RI methodology previously developed (Esnouf et al., 2018) by focusing
451 on the appropriateness of impact categories. We propose a freely downloadable operational tool
452 for RI calculation and have applied this methodology to an illustrative example. The impact
453 category RIs have proven that interpretations of LCIA results can be deepened. They can assist
454 practitioners by orientating their analysis towards relevant impact categories. Analyses were also
455 carried out over all LCI results of the cumulated LCI database to extract global RI trends. The
456 same approach could also be used for other ecoinvent versions, cumulated LCI databases or

457 specific fields of activity. Moreover, the cumulated LCI database trends were used here to
458 standardize the impact categories. Other types of standardization, for example, based on the global
459 elementary flows of a geographical area or economic sector, could relate the RI methodology.
460 Finally, a focus on the standardized elementary flows that provide the value of the impact category
461 RIs for each LCI result could be interesting to trace the main directions that are linked to each
462 impact category.

463 An algorithm proposing a solution for correlation issues was developed and implemented within
464 the operational tool. Redundant information was spread out according to the original impact
465 category RI. Further work could focus on other types of algorithms where the whole impact
466 category subset would not be affected by the modification of RIs. Only the impact categories with
467 elementary flows affected by orthogonalization would be affected. Based on the RI methodology
468 and taking into account the consistency of impact categories, relevant impact categories could also
469 derive from different LCIA methods, thus enabling the development of composite LCIA methods.

470

471 SUPPLEMENTARY INFORMATION AND DATA

472 Supplementary Information A. Additional details for the standardization process and scatter matrix
473 of the ratio $\frac{(RI^{\text{decorr}}-RI)}{RI}$ for the different group of impact categories.

474 Supplementary Information B. An excel file that presents an output example of the Chinese and
475 German LCI result obtained with the python tool-box V.

476

477 CONFLICT OF INTEREST

478 The authors declare no conflict of interest.

479

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483

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