Algorithmically generated subject categories based on citation relations:

An empirical micro study using papers on overall water splitting and related topics

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Abstract

One important reason for the use of field categorization in bibliometrics is the necessity to make citation impact of papers published in different scientific fields comparable with each other. Raw citations are normalized by using field-normalization schemes to achieve comparable citation scores. There are different approaches to field categorization available. They can be broadly classified as intellectual and algorithmic approaches. Recently, a paper-based algorithmically constructed classification system (ACCS) was proposed which is based on citation relations. Using a few ACCS field-specific clusters, we investigate the discriminatory power of the ACCS. The first part of our micro study focusses on papers on overall water splitting. Next, we compare the ACCS with (1) a paper-based intellectual (INSPEC) classification and (2) a journal-based intellectual classification (Web of Science, WoS, subject categories). In the last part of our case study, we also compare the average number of citations in selected ACCS clusters with the average citation count of publications in WoS subject categories related to these clusters. The results of this micro study question the discriminatory power of the ACCS. Thus, we recommend larger follow-up studies on broad datasets.

Key words
Field categorization, bibliometrics, algorithmically constructed classification systems, ACCS, subject categories
1 Introduction

In bibliometrics, it is often necessary to compare the impact of publications from different fields. However, it should be avoided to use bare citation counts (“times cited”) from Web of Science (WoS, Clarivate Analytics) or Scopus (Elsevier) for such comparisons. Many bibliometric studies have shown that there are large differences in citation rates between fields, which cannot be explained by the quality of publications (see, e.g., Bornmann & Marx, 2015). Field-normalized indicators have been developed in bibliometrics which make cross-field comparisons possible. “The idea of these indicators is to correct as much as possible for the effect of variables that one does not want to influence the outcomes of a citation analysis, such as the field … of a publication” (Waltman, 2016, p. 375). The use of normalized indicators in research evaluation is one of the guiding principles for research evaluation in the Leiden manifesto for research metrics (Hicks, Wouters, Waltman, de Rijcke, & Rafols, 2015).

In recent years, several methods have been proposed for the calculation of normalized citation scores. An overview of these methods can be found, for example, in Mingers and Leydesdorff (2015), Waltman (2016), and Bornmann and Marx (2015). Today, indicators based on the idea of counting highly cited publications are seen as a robust method for measuring citation impact across fields (Wilsdon et al., 2015). An important topic in the calculation of field-normalized indicators is the way in which research fields are defined, i.e. which field-categorization schema is used in bibliometrics to calculate the expected number of citations (Wilsdon et al., 2015). The results of bibliometric studies are also dependent on the used schema. The most common approach in bibliometrics is to work with subject categories defined by Clarivate Analytics in WoS or by Elsevier in Scopus. These subject categories are based on sets of journals publishing research from similar areas. However, the use of journal sets for field-normalization is heavily criticized. The most critical point is papers published in multi-disciplinary journals which cannot be assigned to corresponding
fields using journal sets (Hui, 2015; Kronman, Gunnarsson, & Karlsson, 2010). Alternative
approaches which can be used instead of journal sets have been classified by Wang and
Waltman (2016) in mono-disciplinary and multi-disciplinary classification systems.

A mono-disciplinary classification system “covers publications in one particular
research area and usually provides a classification at a relatively high level of detail” (Wang
& Waltman, 2016, p. 348). Mono-disciplinary classification systems, as the Physics and
Astronomy Classification Scheme (PACS) system used in this study, are mostly expert-based
approaches (Wang & Waltman, 2016) where experts in the fields (at least the authors of a
paper) assign papers to corresponding subject categories. PACS is included in the broader
classification scheme of the INSPEC database. At the highest hierarchical level, INSPEC
features the sections A (Physics), B (Electrical Engineering & Electronics), C, (Computers &
Control), and D (Information Technology) (The Institution of Electrical Engineers, 1992).
The section A of INSPEC is identical with PACS.

Recently, Waltman and van Eck (2012) introduced a method for algorithmically
constructing classification systems (ACCS) at the level of individual publications. The
method is a multi-disciplinary classification system and is based on citation relations between
publications. The approach which is explained in more detail in section 2 plays a prominent
role among the available schemes, because it is used in the Leiden ranking (a university
ranking based on bibliometrics, available at http://www.leidenranking.com/) for the
calculation of field-normalized impact scores. In this case study, we investigate the ability of
the method to reliably assign publications to fields. This study is not intended to undertake a
broad comparison between ACCS and other field classification systems, but focus as a micro
study on one field, namely “overall water splitting”, in more detail. The use of this field has
two advantages: (1) The publications can be reliably compiled in WoS by a simple topic
search. (2) One of the labels for a cluster in ACCS is “overall water splitting” (cluster 3.7.3).
Research on overall water splitting is important for hydrogen gas production from water. The
direct water splitting using solar cells or other renewable energy sources is especially appealing.

In the empirical part of this study, we investigate the spread of publications found by the WoS topic search over the ACCS clusters: Are most of the “overall water splitting” publications assigned to cluster 3.7.3? Then, we take the other way around and study the spread of publications in the ACCS cluster “overall water splitting” over WoS and PACS subject categories (SCs). Finally, we compare the ACCS cluster 3.7.3 with its neighboring clusters (3.7.2 and 3.7.4) to investigate the discriminatory power of the ACCS and study citation impact differences of the papers in these neighboring clusters. Papers assigned to different clusters should differ in terms of content as well as citation impact although they are neighboring clusters. The clusters on the same hierarchical level are ordered by the number of papers in the cluster.

2 Field classification systems used in this study

Science is structured by disciplines (e.g. physics or chemistry), whereby each discipline is a specific domain of particular research traditions including paradigms, codes of practice, and methods (Ziman, 1996). Although it is practically impossible that a scientist is not located in at least one discipline, the disciplines are rather loosely organized – as an “invisible college” (Andersen, 2016). Scientific publications are the main research outcome of scientists. The loosely organized disciplines might be one of the main reasons why it does not exist an established and widely accepted field categorization scheme for scientific papers. The two most important multidisciplinary literature databases used for bibliometric purposes (e.g. field normalization) are the WoS and Scopus (Wang & Waltman, 2016; Wouters et al., 2015). The around 250 WoS SCs (such as biochemistry or condensed matter physics) are based on journal sets. Thus, each paper in WoS is assigned to one category or more based on the
assignment of the publishing journals to the WoS SC. The problems of using the WoS SC for field-normalization in bibliometrics are explained by Haddow and Noyons (2013) in detail.

PACS is a mono-disciplinary classification system which was developed by the American Institute of Physics (AIP). PACS classifications are assigned to papers by the authors themselves. According to Radicchi and Castellano (2011) “this guarantees an optimal classification into fields, overcoming the nontrivial problem of attributing, a posteriori, papers to fields. PACS codes are composed of three fields XX.YY.ZZ, where the first two are numerical (two digits each) and the third is alphanumerical. For our purpose we consider only the first digit of the XX code, which provides a classification into very broad categories”.

Other classification systems of professional databases are Chemical Abstract (CA) sections offered by the Chemical Abstract Service (CAS) (Bornmann & Daniel, 2008) and Medical Subject Heading (MeSH) terms by the United States National Library of Medicine (Leydesdorff & Opthof, 2013).

The ACCS developed by Waltman and van Eck (2012) is based on a transparent clustering technique which assigns papers to field-specific clusters based on direct citations between single papers. The algorithm needs three basic parameters as input besides the direct citation network: (1) the number of levels of the classification system. Using only one level results in a non-hierarchical classification system. (2) The resolution parameter determines how much detail is offered at each level. The resolution parameter is bound between 0 and 1. (3) The minimum number of publications per cluster needs to be specified, too. The latter two parameters can have different values for each level of the classification system. The ACCS has four important advantages: (1) The classification works on the level of single publications and not journals (like the WoS scheme). Thus, the assignment of publications to fields is more detailed and difficulties with multidisciplinary journals are avoided. (2) Each paper in the literature database is assigned to a field only once. Usually, field classification systems (e.g. WoS and Scopus journal sets or expert-based systems, such as PACS and CA sections) assign
papers to more than one field which complicates the statistical analysis and the calculation of field-normalized indicators because different counting methods can be applied, e.g., fractional counting, (scaled or unscaled) full counting, and multiplicative counting (Haunschild & Bornmann, 2016). (3) The ACCS is not restricted to a single discipline (such as PACS). Thus, it can be applied to the entire literature database (WoS). (4) The ACCS methodology for the clustering of publications in literature databases is freely available. Thus, the ACCS can be implemented in every in-house literature database which includes direct citation links between publications.

The ACCS methodology is based solely on direct citation links between publications. Thus, frequently used other techniques, such as co-citations, bibliographic coupling, shared words in titles or abstracts, are not part of this methodology. Since there are large differences in citation density between fields (Marx & Bornmann, 2015), Waltman and van Eck (2012) corrected these differences by normalizing relatedness scores by fractional citation counting. Within the ACCS approach of clustering papers, a large-scale optimization problem was solved by introducing the so-called smart local moving algorithm (Waltman & Eck, 2013) which is freely available at www.ludowaltman.nl/slm. This approach is able to handle very large datasets: In the first application of their approach, Waltman and van Eck (2012) classified many millions of papers from the sciences and social sciences published between 2001 and 2010. The received classification system distinguishes between three granularity levels with a minimum of 120,000, 5,000, and 50 papers per cluster. The three levels are hierarchically ordered in the sense that level 1 clusters are nested in level 2 clusters which are themselves clustered in level 3. In such a classification system with three levels, each cluster will be referred to as X.Y.Z where X, Y, and Z are natural numbers. In non-hierarchical classification systems, only one natural number is used to refer to an individual cluster.

Although the ACCS offers many advantages compared to other existing classification systems, it has been criticized. Leydesdorff and Milojević (2015) summarize the critique as
follows: “Because these ‘fields’ are algorithmic artifacts, they cannot easily be named (as against numbered), and therefore cannot be validated. Furthermore, a paper has to be cited or contain references in order to be classified, since the approach is based on direct citation relations. However, algorithmically generated classifications of journals have characteristics very different from content-based (that is, semantically meaningful) classifications … The new Leiden system is not only difficult to validate, it also cannot be accessed or replicated from outside its context of production in Leiden” (p. 201).

3 Datasets used

In this study, we used three datasets:

(1) We use the WoS search query ‘TS=(overall AND ”water splitting”) AND PY=2001-2010’ within the indices Science Citation Index Expanded and Conference Proceedings Citation Index- Science refined to the document types article, letter, and review. This topic search yields many papers from the research on direct water splitting by solar cells. At the date of search (July 5th, 2017), we found 145 records in the WoS. For 144 of the records, we were able to match them with the ACCS clusters via the WoS UTs. We downloaded the classification system which was described in the previous section from http://www.ludowaltman.nl/classification_system/ on November 7th, 2014.

(2) Waltman and van Eck (2012) have provided labels for the ACCS clusters. One of the labels for cluster 3.7.3 is “overall water splitting”. The other labels are “bivo4”, “solid state reaction method”, “sacrificial agent”, and “photocatalytic h”. BiVO4 seems to occur often enough in titles and abstracts of papers in this cluster to appear as one of the labels. However, chemical compounds are not useful field classifications because they are studied in different fields with different foci. The label “photocatalytic h” is rather redundant to “overall water splitting” as water splitting is usually performed via photocatalytic methods. The labels “solid state reaction method” and “sacrificial agent” are also not helpful because these terms
are too broad to use them for field classification. We were able to match all papers (n=1739) of the cluster 3.7.3 via the WoS UTs with their WoS SCs, but only 686 (39.4%) papers could be matched via the DOI with their INSPEC categories in STN (an online database for physics and related areas, see http://www.stn-international.de). The INSPEC classification system was reduced to the second level to be comparable with the ACCS. Papers with more than one classification are counted multiple times in the WoS and INSPEC schemes.

(3) We compare the papers of cluster 3.7.3 with the neighboring clusters 3.7.2 (n=2645 papers) and 3.7.4 (n=1677 papers). The labels of cluster 3.7.2 are “n doped tio2”, “n doping”, “nitrogen”, “tio2 lattice”, and “tio2 xnx” and the labels of cluster 3.7.4 are “catalyst loading”, “initial dye concentration”, “operational parameter”, “azo dye”, and “decolorization”. The labels of cluster 3.7.2 seem rather redundant. We would expect papers about TiO₂, its lattice, and nitrogen doping of TiO₂ in this cluster which is only partly a useful field classification because such aspects are investigated in different scientific fields (e.g., physical chemistry, analytic chemistry, condensed matter physics). The labels of cluster 3.7.4 indicate that this cluster contains papers about azo dyes and catalysis. All papers from the neighboring clusters could be matched via the WoS UTs with their WoS SC. Also, for all papers in the three clusters the citations are determined (from publication year until the end of 2014).

4 Results

Figure 1 shows the distribution of the publications found by the WoS topic search (data set 1) across ACCS clusters. The 144 publications are assigned within the ACCS to 20 clusters. The blue bars show the absolute and the red dots the cumulative relative numbers of papers for each ACCS cluster. 63.9% (n=92) of the papers of our topic search were found in the cluster 3.7.3. Two other clusters 3.26.7 and 2.23.1 contain more than 5% of the topic search results. The labels of ACCS cluster 3.26.7 are "high temperature gas", "hydrogen
production", "htgr", "thermochemical cycle", and "sulfur iodine". The labels of ACCS cluster 2.23.1 are "mn cluster", "oec", "water oxidation", "mu o", and "y z". Although "hydrogen production" and "water oxidation" have considerable thematic overlap with "water splitting", they also deal with different topics. The other labels of the ACCS clusters 3.26.7 and 2.23.1 either apply to different topics or are not helpful (e.g., "htgr" and "y z").

Figure 1: Distribution of the publications found by the WoS topic search for our topic search (data set 1) across ACCS clusters. The blue bars show the absolute numbers of publications in ACCS clusters (y-axis on the left) and the red dots the cumulative relative numbers (y-axis on the right).

The ACCS cluster 3.7.3 contains 1739 papers in total. Only 92 papers (5.3%) in the ACCS cluster 3.7.3 seem to be relevant for the topic of "overall water splitting". Still, it is one of the five most important terms according to the ACCS methodology. One of the other four labels ("photocatalytic h") is rather redundant to "overall water splitting".

Figure 2 shows the distribution of the papers in ACCS cluster 3.7.3 across the INSPEC (n=686 papers) and WoS SCs (n=1739 papers). The blue bars present the distribution across
the INSPEC SCs and the red bars the distribution across the WoS SCs. The figure shows that the cluster 3.7.3 contains papers which are categorized in very different scientific fields (e.g., “Electrochemistry”, “Chemistry, Inorganic & Nuclear” as well as “Electronic transport in condensed matter”, and “Optical properties, condensed matter spectroscopy and other interactions”) in both, the INSPEC and WoS classification systems.

Figure 2: Distribution of the papers in cluster 3.7.3 across the INSPEC and WoS classification systems (in absolute numbers)

In the final step of the analysis, we compare three neighboring ACCS clusters: 3.7.2, 3.7.3, and 3.7.3. The ACCS orders clusters in the same hierarchical level by size (number of papers in the cluster).
Figure 3: Semantic maps of title words of the papers in clusters 3.7.2, 3.7.3, and 3.7.4
Figure 3 shows semantic maps based on a title word analysis of the three clusters. The maps have been produced by using VOSviewer 1.6.5 (www.vosviewer.com). A minimum of 10 occurrences per title word was required in VOSviewer. Although the labels of clusters 3.7.2, 3.7.3, and 3.7.4 are rather different, the title word maps of the papers in these three clusters seem rather similar. For example, Figure 3 shows many terms related to photocatalytic activity and TiO$_2$ in all three clusters as pronounced terms. Judging from the semantic maps, clusters 3.7.2, 3.7.3, and 3.7.4 should belong thus to the same cluster (scientific field).

However, clusters 3.7.2 and 3.7.3 seem to have more similar characteristics (showing the terms synthesis and preparation) in the semantic maps than cluster 3.7.4 (showing the term degradation more prominently). This pattern is further checked using WoS SCs in Figure 4 where the distribution of the ACCS clusters 3.7.2, 3.7.3, and 3.7.4 across SCs is shown. The figure reveals that the papers in clusters 3.7.2 and 3.7.3 distribute more similarly across the WoS SCs than the papers in cluster 3.7.4. For example, about 24% of the papers in cluster 3.7.2 and 27% in cluster 3.7.3 are assigned to “Chemistry, Physical”; the percentage for cluster 3.7.4 is only about 17%. Thus, the distribution across WoS SCs is consistent with the pattern which we observed in the semantic maps in Figure 3.
Figure 4: Distribution of the papers in clusters 3.7.2, 3.7.3, and 3.7.4 across WoS subject categories (in percentages)

The greater similarity of clusters 3.7.2 and 3.7.3 compared to 3.7.4 is also reflected in the mean citation counts of the papers, see Table 1. Table 1 summarizes the number of papers and the average citation count for the three investigated ACCS clusters. The difference in citation counts between clusters 3.7.2 (avg. TC=52.91) and 3.7.3 (avg. TC=46.09) is 6.82 compared to (1) 13.08 for clusters 3.7.3 and 3.7.4 (avg. TC=33.01) and (2) 19.9 for clusters 3.7.2 and 3.7.4.

Taken together, although two clusters are more similar to one another than the third cluster to both, the results are contrary to algorithmically constructed fields with high discriminatory power.

Table 1: Number of papers and average citation counts (average times cited, avg. TC) for the three studied ACCS clusters
| ACCS cluster | Number of papers | Avg. TC |
|--------------|------------------|---------|
| 3.7.2        | 2645             | 52.91   |
| 3.7.3        | 1739             | 46.09   |
| 3.7.4        | 1677             | 33.01   |

Figure 5 shows the average citation counts for all papers assigned to the WoS SCs from Figure 4. It is based on all papers published between 2001 and 2010. The WoS SCs in Figure 5 are ordered by the number of papers also assigned to ACCS cluster 3.7.3 as in Figure 4. We would like to compare these citation counts with the average citation counts in Table 1. The difference between both figures is that the citation counts in Figure 4 are restricted to the papers belonging to the three clusters and those in Figure 5 refer to all papers in the SCs. Citation impact on a similar level would reveal similarities between WoS SCs and the three clusters. As the results in Figure 5 reveal, however, the average citation counts of the papers in the WoS SCs vary between 5 and 25 citations per paper whereas the average citation counts in Figure 4 for the clusters 3.7.2, 3.7.3, and 3.7.4 are 33.01, 46.09, and 52.9 citations per paper, respectively. Obviously, the clusters contain papers with significantly higher average citation counts than the papers in the corresponding WoS subject categories.
Discussion

Using papers on “overall water splitting”, we have compared the ACCS with two other SC systems (PACS and WoS). Our study follows the recommendation of Waltman and van Eck (2012) for doing such studies: “Another approach may be to compare the results of our methodology with existing publication-level classification systems such as the Physics and Astronomy Classification Scheme (PACS)” (p. 2390). We started the comparison with all papers found using the WoS topic search “overall water splitting”. The results show that about 64% of the papers are assigned to the ACCS cluster 3.7.3 which has the label “overall water splitting” besides other labels. Many papers are spread over many other ACCS clusters. In a second analysis, we used all papers in the ACCS cluster which has “overall water splitting” as one label. The results reveal that these papers are assigned to many different
WoS and INSPEC categories. The further comparison of cluster 3.7.3 with its neighboring clusters on the basis of semantic maps and citation counts questions the discriminatory power of the ACCS.

One possible interpretation of our results is that the cluster algorithm used to construct ACCS is not able to distinguish properly between scientific fields. This interpretation is confirmed by similar results which have been published by Rafols and Leydesdorff (2009). They compared content-based and algorithmic classifications of journals (Leydesdorff & Milojević, 2015). One should have in mind in the comparison of field classification systems and in the interpretation of the results of this study, however, that “the idea of science being subdivided into a number of clearly delineated fields is artificial. In reality, boundaries between fields tend to be rather fuzzy” (Waltman & van Eck, 2013, p. 700). Thus, a completely satisfying solution seems to be impossible. Although the results of this study and Rafols and Leydesdorff (2009) point out that caution should be exercised when normalized indicators based on the algorithmic classification system are used, the results of Perianes-Rodriguez and Ruiz-Castillo (2015) for the Leiden Ranking show that normalized impact values for universities are highly correlated if they are calculated using the WoS SCs or ACCS, respectively.

We assume that the results by Perianes-Rodriguez and Ruiz-Castillo (2015) are mainly due to the aggregation level of universities included in the Leiden Ranking. The results of our study indicate that changes in the field classification system affect the mean citation impact significantly. The normalized impact indicators for a paper (or paper set) are not comparable when they are calculated using different classification schemes. The average citation counts which we calculated for WoS SCs and ACCS clusters are so different that they will result in different normalized impact scores if used as reference sets. Since there is no preference in bibliometrics for one or another classification system, both are equally in use. It is an advantage of the ACCS that it makes the work of bibliometricians easier, because it contains
no multiple classifications of papers. The disadvantage is that research evaluation based on ACCS is not transparent because clusters cannot be labelled properly and can contain (depending on the cluster resolution) too many different research fields in a single cluster or research fields are split artificially into different clusters.

Since this micro study is based on the papers on only one topic, it is unknown if the results can be generalized. However, one example is enough to point to a general flaw in an algorithm. Further studies should follow with comparisons on other subject-specific databases with broad coverages of related subject areas and preferably intellectual assignments of scientific fields to publications. Future studies should consider as many available proposals as possible in the bibliometric literature for field delineations. An overview can be found in Wouters et al. (2015).
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