# "Structuration" by Intellectual Organization: The Configuration of Knowledge in Relations among Scientific Texts

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## Abstract

Using aggregated journal-journal citation networks, the measurement of anticipation in empirical systems is examined in two cases of interdisciplinary developments during the period 1995-2005: (i) the development of nanotechnology in the natural sciences and (ii) the development of communication studies as an interdiscipline between social psychology and political science. The results are compared with a case of stable development: the citation networks of core journals in chemistry. The textual networks are intellectually organized by networks of expectations in the knowledge base at the specialty (that is, above-journal) level. This "structuration" of structural components in the observable networks can be measured as configurational information. The latter can be compared with the Shannon-type information generated in the interactions among structural components: the difference between these two measures provides us with a redundancy generated by the specification of a model in the knowledge base of the system. The knowledge base incurs to variable extents on the knowledge infrastructures provided by the networks of exchange relations.

**Keywords**: meaning, knowledge, dynamics, configuration, redundancy, synergy, journal, citation.

## Introduction

Knowledge can be considered as a meaning that makes a difference in terms of a code of communication developed within a system of relations. The code can be embodied, as in the case of an individual, or it can be reproduced in a network of relations. In the latter case, *discursive* knowledge can be developed at the network level. While it is common to consider agents as knowledgeable, the concept of knowledge stored in or processed by networks requires explanation. The knowledge carried by a network is more than and different from the sum of the knowledge carried by individual agents. For example, codified knowledge has been considered as a common good in evolutionary economics (Dasgupta & David, 1994).

Networks can develop as structures in different dimensions that recursively condition and enable further developments. Thus, differentiation (at each moment of time) and path-dependencies potentially involving restructuration (over time) can be expected. From an evolutionary perspective, networks of relations can be considered as the historical retention mechanisms of flows of communication through the networks. These flows of communication are structured by codes of communication (Leydesdorff, 2007).

Functional differentiation among the codes of communication enables a networked system to process more complexity (Luhmann, 1986; 1995; Simon, 1972). The functions can be expected to develop evolutionarily in terms of the structural dimensions of the networks (eigenvectors), while the networks of relations develop historically in terms of

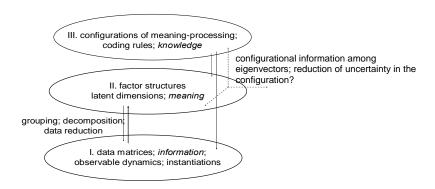
(aggregates of) relations. The network is constructed bottom-up, but the codes of communication feed back as a top-down control mechanism. Note that different topologies are involved: relations are discrete events in design space, but the eigenvectors span a function space with continuous dimensions (Bradshaw and Lienert, 1991; Simon, 1973). The eigenvectors can be expected to change with a dynamics different from those of the networks of observable relations. A "duality of structure" is generated because the events take place in two concurrent spaces (Giddens, 1979).

From a systems perspective, structural components can be considered as condensations of the different functions carried by a networked system. The densities are reproduced because they are functional. However, a knowledge-based system adds an overlay on top of the differentiation in an attempt to integrate the different perspectives using a model. This model "structurates" the configuration of eigenvectors—with reference to other possible configurations—whereas the eigenvectors provide structure to the observable variation. Furthermore, a model gives meaning to the modeled system. In a networked system different models can be exchanged and discursive knowledge generated as an interaction term in addition to and on top of the sum total of reflexive models at the level of each individual agent.

A system which entertains a model of itself can be considered as anticipatory (Rosen, 1985; Dubois, 1998). Different models can be entertained in a network system.

Discursive knowledge at the level of the social system originates from the updates of models among reflexive agents in mutual contingencies (Parsons, 1968; Strydom, 1999;

Vanderstraeten, 2002). This intersubjective updating among models adds another anticipatory dynamic to the anticipatory dynamic at the level of individual systems. The two anticipatory dynamics—the one within each individual system and the other caused by communication among them—operating upon each other can be expected to generate strong anticipation in a knowledge-based social system (Leydesdorff, 2008, 2009a). Strongly anticipatory systems can be expected to co-construct their future states, as in the case of techno-economic co-evolutions, by structurating the structures in the data using time as another degree of freedom.



**Figure 1**: A layered process of codification of information by meaning, and codification of meaning in terms of a knowledge base.

Figure 1 summarizes this theoretical argument in terms of an empirical research design.

First, observable data matrices can be factor analyzed. The factor model provides structure by reducing the data. As structure develops over time, trajectories can be shaped which stabilize a system. Three selections are involved: (i) the momentary positioning of the data in a multidimensional space of eigenvectors, (ii) the positioning over time in series of events, and (iii) reconstruction in the present on the basis of a reflexive model.

Whereas trajectories develop in terms of the first two selections, the third selection mechanism can be expected to meta-stabilize, hyper-stabilize or globalize trajectories at the regime level (Dosi, 1982; Dolfsma & Leydesdorff, 2009).

In other words, we follow Giddens's (1979, at pp. 66 ff.) distinction between *structure* and *structuration*. While structure can be operationalized in terms of latent dimensions, "structuration" governs the transformation of structures, and therefore the reproduction of a system. Giddens, however, defined a system in terms of reproduced relations, that is, as a network of observable relations (in the design space). From our perspective, the network provides only the instantiations of the system, while communication systems develop operationally in terms of different functions (Luhmann, 1995). The operations should not be reified as network relations: the reflexive overlay does not exist as *res extensa*, but can be considered as an order of expectations in the model (*cogitata*) which potentially feeds back on the observable relations by reducing uncertainty (Husserl, 1929; Luhmann, 2002a). This additional degree of freedom enables the system to self-organize knowledge by selecting from different meanings provided to the information. <sup>1</sup>

In this study, we develop this three-layered model in empirical terms using aggregated citation relations among scientific journals as networks. Scientific journals are organized in functionally different groups. For example, articles in analytical chemistry rarely cite articles in the social sciences, or *vice versa*. Thus, one obtains densities in these networks

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<sup>&</sup>lt;sup>1</sup> Luhmann (1995, at p. 67) used Bateson's (1972, at p. 453) definition of information as "a difference which makes a difference." Shannon-type information is provided by a series of differences contained in a distribution, and remains meaningless before the specification of a system of reference for the measurement.

which are reproduced from year to year for functional reasons. The densities can be considered as representations of the functions (of puzzle-solving and truth-finding) carried by the networks. For example, some journals function to reproduce the specialty of analytical chemistry, while others reproduce sociology. Note that specialized knowledge is produced and retained at the above-journal level of journal sets in specific configurations with exchange relations among them (Lucio-Arias & Leydesdorff, 2009). The observable exchange relations provide the variation; the above-journal relations in a configuration of eigenvectors can be considered as a network of expectations.

An evolving system develops in terms of its structure and not in terms of observable variations. Structural components can be considered as competing selection mechanisms. They provide meaning to the observable events in orthogonal dimensions. In a next step, I shall use the configurations among eigenvectors as an operationalization of "structuration" and measure configurations among structural components using information theory. Animations enable us additionally to visualize the resulting dynamics of the networks. Whether stabilization occurs, however, remains an empirical question even if relations among structural components are indicated at specific moments of time. Furthermore, a next-order dynamics is invoked in the case of structural changes over time; the "structuration" among the components which develops along trajectories is then changed at the regime level of the system. A knowledge-based system rests as a regime of pending selections on the variations, momentary selections, and historical trajectories on top of which it emerges reflexively.

In other words, the events (that is, relations at the network level) are provided with different meanings by each selection mechanism. The variable is first positioned by the factor model in a multidimensional space. The factor model provides a momentary meaning to the variation. Analogously, the variables and eigenvectors develop over time and can be provided with historical meaning along this second axis. Combinations of positional and historical meanings can be evaluated at the systems level in terms of configurations. A meaning which makes a difference at this level of a system's model can be specified as knowledge. The observable uncertainty in the modeled system remains the external referent of this system of expectations. If the structures in the events change over time, the system's knowledge base may be in need of an update.

#### Test cases

We focus on two instances of structural changes in network dynamics that we previously studied in detail: (1) the generation of a network of nanotechnology journals on the basis of a merger of the networks in applied physics and specific chemistry journals around 2000 (Leydesdorff & Schank, 2008), and (2) the emergence of communication studies as a network of aggregated journal-journal citation relations during the last 15 years (Leydesdorff & Probst, 2009). In these two previous studies, animations were generated for the respective fields based on trading off the stress in the representation based on multidimensional scaling at each moment of time against the stress values over time using the dynamic version of *Visone* (Baur & Schank, 2008; Leydesdorff *et al.*, 2008).<sup>2</sup>

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<sup>&</sup>lt;sup>2</sup> The dynamic version of *Visone* is freeware available at <a href="http://www.leydesdorff.net/visone">http://www.leydesdorff.net/visone</a>.

The animation for the nanotechnology journals (available at

http://www.leydesdorff.net/journals/nanotech) first shows the embeddedness of the journal *Nanotechnology* in its relevant citation environment of journals in applied physics during the second half of the 1990s. Increasingly, chemistry journals in the environment were attracted to this focus in terms of citation relations. The journal *Science* played a catalyzing role in merging the two disciplinary frameworks around 2000. Thereafter, a new cluster of nano-journals emerged in which *Science* again played a role, but at this time as one of the specialist journals of the emerging field of nanoscience and nanotechnology. For example, the Institute of Scientific Information (ISI) of Thomson-Reuters added the new subject category *Nanoscience & Nanotechnology* to their database in 2005. At this time, 27 journals could already be subsumed under the new category.

Communication studies—our second case—can be considered as an emerging interdiscipline between mass-communication with roots in political science and interpersonal communication rooted predominantly in social psychology. Rogers (1999, at p. 618) described this division in communication studies as "a canyon" which would be dysfunctional to the further development of the discipline. Leydesdorff & Probst (2009) focused on the delineation of a journal set that would be representative of the emerging inter-discipline.

Using the same techniques as in the study about nanotechnology, we could show that in the citation impact environment (available at

http://www.leydesdorff.net/commstudies/cited) more than in the citing patterns of these

journals, a third density evolved which can be identified as communication studies. Our explanation was, that despite different intellectual origins which lead to different citation patterns from other disciplinary perspectives, this third group of journals is perceived increasingly as a structural component of the network. The eigenvector in the being-cited patterns of the subset of communication journals became gradually more pronounced.

In this study, we take the animation technique one step further, first, by including the three main eigenvectors into the animations. The data is reduced to three factors because three is the lowest (and therefore most parsimonious) number of variables with interaction effects. The mutual information between two variables is always positive (or zero in the case of independence), but the mutual information or, equivalently, the interaction term in a three-dimensional variance can be negative (Garner & McGill, 1956). This measure is also known as interaction information or configurational information (McGill, 1954; Yeung, 2008), and is used pervasively in empirical studies as a measure of interaction among three or more dimensions.

Configurational information has the seemingly attractive property of indicating synergy in the information transfer in terms of negative and positive values (Jakulin, 2005).

However, this information is not a Shannon-measure and therefore has remained difficult to interpret (Watanabe, 1960; Yeung, 2008, at p. 59). Garner & McGill (1956, at p. 225) noted that a negative interaction term in the variance can only be the result of non-orthogonality in the design. Recently, Krippendorff (2009a, at p. 200) argued that circular relationships among the components are then deemed possible, which contradicts

Shannon's assumptions of linear relationships. In Shannon's (1948) theory, the reception of a message cannot feed back on the message sent.

In a further elaboration (Krippendorff, 2009b), configurational information (Q) was identified as the net result of the Shannon-type information flow in the interactions (I) diminished with redundancy (R) in the model specification of these interactions at a next-order systems level. One may wish to follow Krippendorff and consider this next-order level as an "observer," but one should keep in mind that this "observer" is only able to specify a model in terms of expectations. However, the redundancy (R) and, therefore, the configurational information (Q) are *not* a property of the multivariate probability distributions in the modeled system, but their values are contained in them and can be derived from them algorithmically as (potentially negative!) expected information.

In other words, because of the contextualization of the relation by a third variable, the uncertainty in the relation between two variables can be changed (as in the case of partial correlation coefficients). Krippendorff (2009b) distinguished between the additional three-dimensional term using the Shannon-type decomposition ( $I_{ABC \rightarrow AB:AC:BC}$ ) from the configurational information (Q) and from the redundancy (R) originating from the specification, and derived: R = I - Q. One can measure both I and Q in three or more dimensions of the data.

While equally uneasy about the interpretation of configurational information (as not a Shannon measure), Sun & Negishi (2008) compared this indicator with partial correlation

coefficients in an empirical study of Japanese trans-sectoral (university, industry, government) and international coauthorship relations (Leydesdorff & Sun, 2009; Sun *et al.*, 2008). We shall explore this alternative measure as another indicator of configurational effects in addition to mutual information in three dimensions and Krippendorff's ternary information term. In summary, this study tests the model of knowledge generation depicted in Figure 1 against the background of two previous studies about the observable behavior of the journal systems under study.

In a third part of the empirical study, we compare our results for the two case studies (which will indicate only small redundancies at the system level during these transitions) with a case of relatively stable development using the ego-network of citations to the *Journal of the American Chemical Society (JACS)* above a certain (1%) threshold level. This data was studied in previous research projects (Leydesdorff, 1991; Leydesdorff & Bensman, 2006). In this relatively stable case, the relation between the development of structure *versus* system—that is, Giddens's (1979) "duality of structure"—can be shown to operate differently from the two cases of interdisciplinary reorganization.

## Methods and data

Data was harvested from the CD-Rom versions of the *Journal Citation Reports* of the *Science Citation Index* and the *Social Science Citation Index* combined. In the case study about nanotechnology, all journals contributing to the citation impact environment of the journal *Nanotechnology* to the extent of 0.1% or more were included in the analysis in

each year. In the case of communication studies, journal selection was based on the three ISI Subject Categories of "Communication," "Political Science," and "Social Psychology" combined with a Boolean OR-statement.<sup>3</sup> As noted, social psychology and political science can be considered as the two parent disciplines for the inter-discipline of communication studies. Thirdly, in the case of using *JACS* as a seed journal for a relevant citation impact environment, one percent of this journal's total citations are used as a threshold for generating a citation network among approximately 20 (citing) chemistry journals in each consecutive year (1994-2007).

The citation matrices are factor-analyzed in SPSS (v. 15) using a three-factor model. The resulting factor matrices—that is, asymmetrical two-mode matrices—are used as input to  $Pajek^4$  for the visualization and to Visone for the animation.<sup>2</sup> The visualizations position the eigenvectors in the same space as the vectors using the factor loadings (that is, Pearson correlation coefficients) as (normalized) relational indicators. As a threshold, only positive correlations were included in these visualizations.<sup>5</sup>

In other words, the factor loadings on the three main factors are considered as measures of association to the first three hypothesized dimensions of the multidimensional space.  $^6$  Correlations and partial correlations between the three lists of factor loadings can be obtained directly within SPSS. In order to compute configurational information (Q) and

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 $<sup>^3</sup>$  Journals can be multiply assigned by ISI Subject Categories: on average 1.56 ( $\pm$  0.76) categories/journal in 2007 (Rafols & Leydesdorff, forthcoming).

<sup>&</sup>lt;sup>4</sup> Pajek is a network visualization program available at <a href="http://vlado.fmf.uni-lj.si/pub/networks/pajek/">http://vlado.fmf.uni-lj.si/pub/networks/pajek/</a>.

<sup>&</sup>lt;sup>5</sup> Because the dynamic algorithm in *Visone* uses non-metric multidimensional scaling, negative values cannot be distinguished from positive ones. The use of the value r = 0, however, is also convenient as a threshold (Egghe & Leydesdorff, 2009).

<sup>&</sup>lt;sup>6</sup> Factor scores are by definition independent since they represent the projection of the vector on the orthogonal eigenvectors.

Krippendorff's information measure ( $I_{ABC \to AB:AC:BC}$ ) among the three lists of factor loadings, the values are counted in bins ranging from -1 to +1 in ten steps of 0.2. This generates a three-dimensional probability distribution with  $10^3$  (= 1000) cells. Dedicated software was written for the computation of Q and  $I_{ABC \to AB:AC:BC}$ .

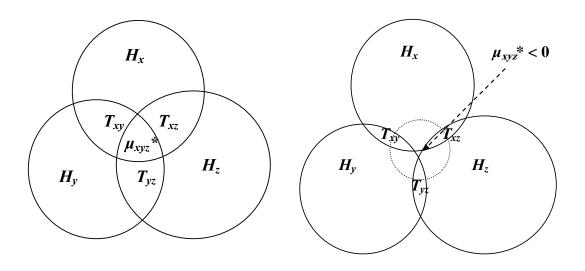
Configurational information  $\mu^*$  (Yeung, 2008, pp. 51 ff.) can be calculated using Abramson's (1963, at p. 129) extension of mutual information in two to three dimensions:

$$\mu_{xyz}^* = H_x + H_y + H_z - H_{xy} - H_{xz} - H_{yz} + H_{xyz}$$
 (1)

Each of the terms in this formula represents a (Shannon) entropy:  $H_x = -\sum_x p_x \log_2 p_x$ ,  $H_{xy} = -\sum_x \sum_y p_{xy} \log_2 p_{xy}$ , etc., where  $\sum_x p_x$  represents the probability distribution of attribute x and  $\sum_x \sum_y p_{xy}$  the probability distribution of attributes x and y combined. The two-dimensional transmission or mutual information  $(T_{xy} = H_x + H_y - H_{xy})$  is zero in the case of two independent distributions, but otherwise necessarily positive. The resulting value of the information measure  $\mu^*$  (Eq. 1) can be positive or negative depending on the relative weights of the uncertainties involved.

McGill & Quastler (1955, at p. 89) proposed calling this measure with the opposite sign a function of partial relatedness  $A = -\mu^*$  because "negative interaction information is produced when the information transmitted between a pair of variables is due to a

regression on a third" (McGill, 1954, at p. 108). The measure is used throughout the literature with both signs: Yeung's (2008, at pp. 51 ff.), aware that this is not a Shannon measure, proposed formalizing  $T_{xyz}$  as the information measure  $\mu^*$ . Krippendorff (2009a and b) followed McGill's (1954) notation, but used Q instead of A. We shall follow Yeung's (2008) and Krippendorff's (2009a) notations, and hence  $Q = -\mu^*$ .



**Figure 2:** Relations between probabilistic entropies (H), transmissions (T), and configurational information ( $\mu^*$ ) for three interacting variables.

Figure 2 provides a metaphorical representation of this information measure based on set theory, which may nevertheless be helpful. If the configurational information  $\mu^*$  is positive (left-hand picture), the third system z receives the same information in the overlap ( $\mu^*$ ) from both x and y. Jakulin (2005) proposed considering this as a redundancy as opposed to a synergy in the right-hand figure. In the right-hand case, the contextualization of the relation between x and y by z allows for the transmission of information via the third system in addition to the direct transmission ( $T_{xy}$ ) between x and y. Thus, the capacity of the channel is changed because of the specification of the model.

Krippendorff (2009b) proposed considering this additional capacity as a redundancy R: uncertainty in the system is reduced by the model specification as a feedback.

From this perspective, the overlap in the left-hand picture adds ternary Shannon-type information ( $I_{ABC \to AB:AC:BC}$ ) which cannot be reduced to its three binary information contents. Q (=  $-\mu^*$ ) measures the difference between the redundancy specified by the model at the systems level and the Shannon-type information generated by the interaction. Hence: R = I - Q (or equivalently,  $R = I + \mu^*$ ). I and Q can be measured, and the redundancy generated by the model specification (R) can therefore be derived.

The model is specified by an observer in first-order cybernetics or by a system observing itself in second-order cybernetics (e.g., Von Foerster, 1982). In the latter case, the next-order level can perform like a hyper-cycle, as indicated in Figure 2 with a dotted line. The hyper-cycle enables the system to observe the expected information content from all (orthogonal) perspectives, and thus to integrate a model. The resulting model operates with a potentially negative feedback on the necessarily positive generation of Shannon-type information. If the negative feedback term prevails, self-organization is indicated as an endogenous reduction of uncertainty in the system.

Ulanowicz (1986, at pp. 142 ff.) proposed using the potentially negative value of mutual information in three dimensions as an indicator of self-organization, that is, the net result of forward information processing and the modeling of this information processing at a

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<sup>&</sup>lt;sup>7</sup> The second law of thermodynamics holds equally for probabilistic entropy, since  $S = k_B H$  and  $k_B$  is a constant (the Boltzmann constant). The development of S over time is a function of the development of H, and *vice versa*.

next-order level within a system (Leydesdorff, 2009b). If a model is generated *within* a system as in an anticipatory system (Rosen, 1985; Dubois, 1998; Leydesdorff, 2009a) or autopoietically (Maturana, 1978; Maturana & Varela, 1980), this model provides meaning to the history of the system from the perspective of hindsight, that is, against the arrow of time. This potentially reduces uncertainty within the system, but as a negative component in an otherwise increasing uncertainty. The next-order level can be that of an external (super-)observer or a set of models using different perspectives entertained in and by a networked system.

The specification of Krippendorff's (2009a) ternary information interaction term  $I_{ABC \to AB:AC:BC}$  in bits of information can be achieved by comparing the system's state to the maximum entropy of the probability distribution. With his kind assistance I was able to reproduce Krippendorff's (1986, at p. 58) algorithm for the computation (cf. Krippendorff, 2009a, at p. 200). This routine is available at <a href="http://www.leydesdorff.net/software/krippendorff/index.htm">http://www.leydesdorff.net/software/krippendorff/index.htm</a>. The algorithm was further extended from the binary case to the decimal one. In other words, I used the algorithm on the same probability distribution of  $10 \times 10 \times 10 = 1000$ ) probabilities as was used for the computation of the configurational information. Both  $Q = -\mu$  and  $I_{ABC \to AB:AC:BC}$  are expressed in bits. Therefore, the R = I - Q of the model is also expressed in bits of information.

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<sup>&</sup>lt;sup>8</sup> Krippendorff's original program (in Fortran) can be retrieved from <a href="http://www.pdx.edu/sysc/research-discrete-multivariate-modeling">http://www.pdx.edu/sysc/research-discrete-multivariate-modeling</a>.

#### Results

While the above mentioned animations of the networks among journals allow us to visualize the emergence of new structural components, the animations with the eigenvectors embedded in these networks enable us to appreciate changing configurations among the components. The animations for the two fields under study with the eigenvectors embedded are brought online at

http://www.leydesdorff.net/eigenvectors/nanotechnology and http://www.leydesdorff.net/eigenvectors/commstudies, respectively.

The bi-modal factor matrices are represented in two colors: green for the eigenvectors and red for the variables, that is, the aggregated citation patterns of the journals that form the networks. In the animation of the group of nanotechnology-relevant journals, journals with "nano" in their title are indicated in blue, while the node representing the journal *Science* is colored pink. In the animation of journal relations in the environment of communication studies, the 28 journals that were attributed to communication studies in 2007 by Leydesdorff & Probst (2009) are colored blue so that one can follow the emergence of this cluster.

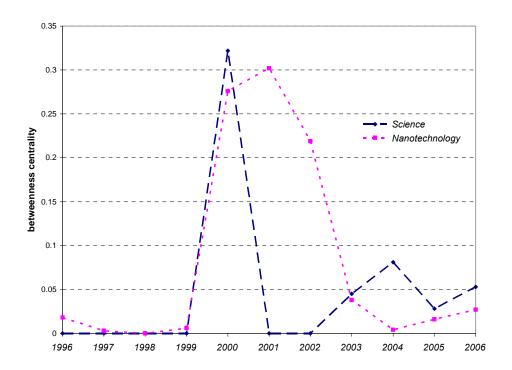
## a. Nanoscience and nanotechnology

The animation of the eigenvectors indicates a reorganization of structural components during the period under study. When the journal *Nanotechnology* entered the database in

1996, it was part of a structure of journals with a focus on "Applied Physics". This first eigenvector relates to a second one which we designated as "New Materials" because in addition to chemistry journals, journals in the life sciences also load on this factor. The third factor is not easy to designate in this year (1996), but is also firmly embedded in the physics domain.

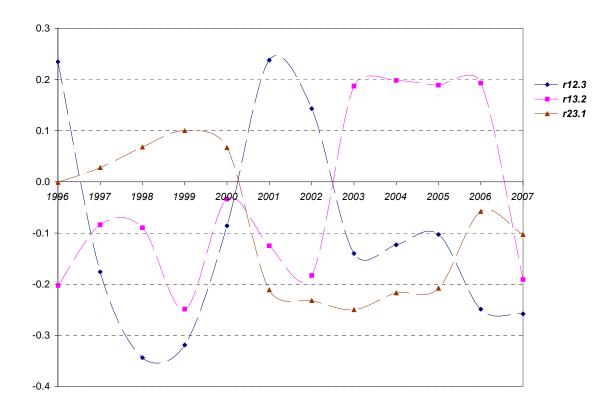
From 1997 onwards, the third factor can be designated unambiguously as "Chemistry". The journal Science takes part in this citation network, but mainly in relation to the chemistry factor. The journal Nanotechnology relates to "Applied Physics" more than "New Materials". In 1999, the factors "Chemistry" and "New Materials" become increasingly related. Science relates positively to all three factors, and Nanotechnology has shifted to a position more central in the map, by relating also to "New Materials".

In 2000, the relations among the disciplinary fields are reorganized; both *Science* and *Nature* participate in this reorganization. This leads to a much closer connection between "Applied Physics" and "New Materials", while the journal Nanotechnology relates both these fields to "Chemistry". New journals with the root "nano" in their title emerge in the transition from 2001 to 2002, among them the journal Nano Letters published by the influential American Chemical Society. A triangle emerges among the three eigenvectors during the years thereafter with the nano-journals located centrally within it. The factor "New Materials" remains more closely related to "Applied Physics" than to "Chemistry".



**Figure 3**: Betweenness centrality in the vector space for the journals *Science* and *Nanotechnology* during the period of the transition (cf. Leydesdorff & Schank, 2009, at p. 1816).

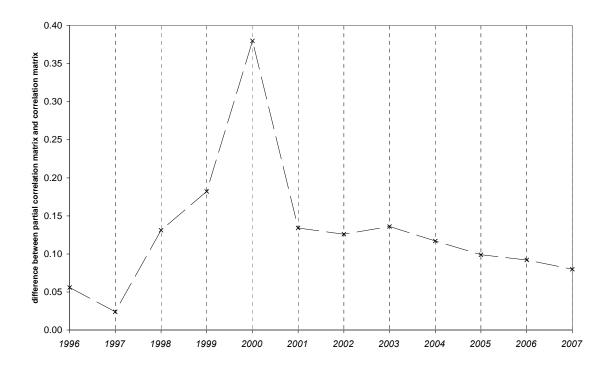
Leydesdorff & Schank (2008) provided a similar account of this development at the level of journals, but not of fields. The transition was indicated by the increasing and decreasing betweenness centrality of the seed journal *Nanotechnology*, which peaked in 2001. In Figure 3, betweenness centrality of *Science* is added, with a peak in 2000. *Nanotechnology* took the role at the interface over from *Science* in 2001. As noted, in the years thereafter other journals were published in this same field. Would one be able to indicate the restructuration among the disciplines as taking place in 2000 using an operationalization at the field level?



**Figure 4**: Partial correlation coefficients among the three main factors in the case of nanotechnology.

Figure 4 shows the development of the partial correlations coefficients among the three factors during the decade under study. As noted above, the factor designation is not always the same among these first three categories, but here the focus is on how the reorganization among them is represented. The reorganization is indicated as a reorganization of the three partial correlation coefficients between 2000 and 2001. The configuration remains unstable in the two years thereafter, but seems to gain more stability from 2003 onwards. The change in the position of *Science* in 2000 is evaluated as a non-structural variation from this perspective: the development at the level of journals did not yet affect the factor structure in 2000, but did so by 2001.

The partial correlation coefficients are significantly correlated to the Pearson correlation coefficients (r = 0.948; p < 0.01). Actually, the two figures would be virtually similar, but using the Pearson correlation coefficients, the emphasis in the reorganization shifts from the first crossing of values between 2000 and 2001 towards the second one between 2002 and 2003. This result supports Sun & Negishi's (2008) argument for using the partial correlation coefficients.

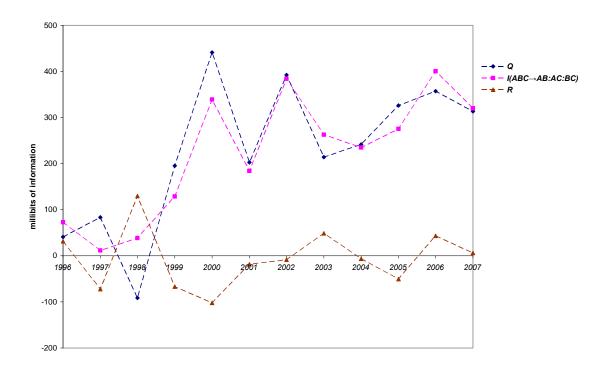


**Figure 5**: Sum of differences between the Pearson correlations and the partial correlation coefficients for different years.

The difference between the two matrices is shown in Figure 5 as the sum of the absolute differences between the corresponding cell values in the two matrices. The figure

highlights the change taking place in 2000. However, this indicator remains conceptually an ad-hoc measure, although it shares with configurational information that the effect of contextualization in a third dimension is indicated as a difference.

Let us turn to the information measures where this difference between structure and system can be defined as Q = I - R. Figure 6 shows the development during this period of configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R in millibits of information. Table 1 presents this data in tabular format.



**Figure 6**: The configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R = I - Q in millibits of information for the case of nanotechnology.

	Q	I <sub>ABC→AB:AC:BC</sub>	R	Ν
1996	41	73	32	41
1997	83	11	-72	45
1998	-91	39	130	51
1999	196	129	-67	69
2000	441	339	-102	72
2001	203	184	-18	99
2002	392	384	-8	114
2003	214	263	49	167
2004	241	235	-6	172
2005	326	275	-50	140
2006	357	401	43	140
2007	313	320	6	160

**Table 1**: The configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R = I - Q in millibits of information for the case of nanotechnology.

Figure 6 shows that both measures register the change in the configuration in 2000 with precision. The two measures are marginally different both in absolute values and in their development patterns (r = 0.913; p < 0.01), and consequently R is small. In other words, if R is considered as the feedback term from the intellectual (self-)organization of the field surrounding the journal *Nanotechnology* as its citation impact environment, this intellectual organization is notably in disarray in 2000, but is also not stable in the other years under study. Perhaps, this is a consequence of the bias introduced by focusing on a single journal and its environment. In the next study, we therefore turn to a development defined at the level of (inter-)disciplines operationalized as groups of journals in the same subject categories as defined by the Institute of Scientific Information (ISI).

## b. Communication Studies

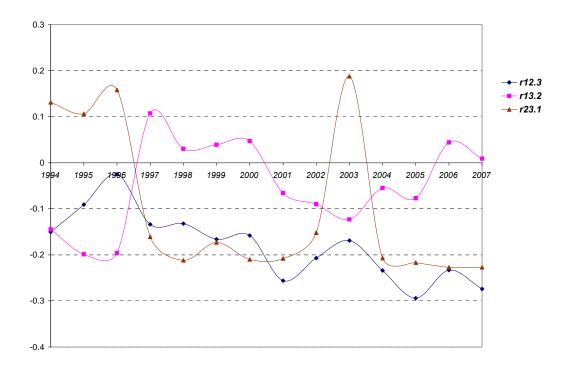
Inspection of the citation impact patterns of the individual journals (at <a href="http://www.leydesdorff.net/commstudies/cited">http://www.leydesdorff.net/commstudies/cited</a>) shows a third density increasingly emerging in addition to journals in social psychology and political science, which themselves form dense network components. A precise transition from a loose network to a structural component in the third dimension, however, is not clearly indicated. Upon visual inspection, the development seems mainly gradual. Is it possible to indicate structural change in this development?

In the years 1994-1996, the journal *Public Opinion Quarterly* played a key role in relating the communication studies journals first to journals in the political sciences, and then also to journals in social psychology. The years 1996-1998 witnessed notably an increase in the density of relations between communication studies and social psychology. In 1998, *Public Opinion Quarterly* and *Human Communications Research* were central to the interfaces of the emerging cluster of journals in communication studies with journals in political science and social psychology, respectively.

In terms of eigenvector development, the communication studies journals were first (1994-1995) immersed in the internal complexity of two factors (Factors Two and Three) which can both be designated as political science. One of these factors focuses on political units of analysis such as comparisons among nation states, and the other more on political processes, led by American journals (such as the *American Political Science* 

*Review* and *American Political Quarterly*). The communication studies journals load negatively on the former of these two factors, but neutrally on the latter.

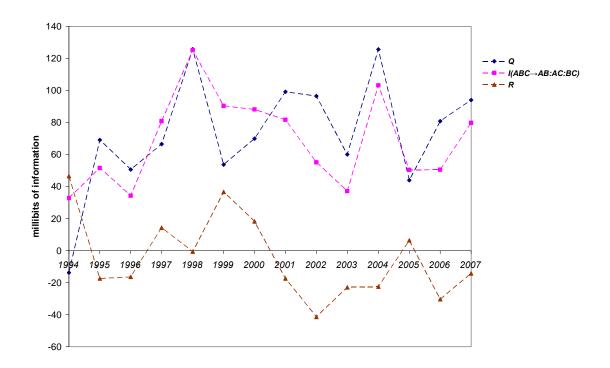
In 1996, this profile is enhanced: both the *Journal of Communication* and *Communication Research*—two flagship journals of the International Communications Association (ICA)—load negatively (with –0.641 and –0.630, respectively) on a factor that is otherwise still dominated with a positive sign by journals such as the *European Journal of Political Research*, the *British Journal of Political Science*, and *Election Studies*. This third factor is a mixture of the two components in this year preceding the transition. In 1997, however, the third factor can be designated unambiguously as "*Communication Studies*" in addition to a first factor representing "*Social Psychology*" and a second "*Political Science*". (The American journals mentioned above dominate this latter factor, but the other group is part of it given a three-factor model.)



**Figure 7**: Partial correlation coefficients among the factor loadings on three main factors in the case of communication studies.

Figure 7 indicates the changes: the partial correlations of the loadings on both Factors One (social psychology) and Two (political science) with Factor Three change sign between 1996 and 1997. The third factor groups a set of journals in communication studies in the latter year for the first time. The other major event indicated, is the disappearance of the (third) communication-studies factor in 2003. In this year only, the pre-1997 configuration is restored for a single year. This effect in 2003 is also visible in the animation (at <a href="http://www.leydesdorff.net/eigenvectors/commstudies/">http://www.leydesdorff.net/eigenvectors/commstudies/</a>).

The partial correlations are in this case even more strongly correlated to the Pearson correlations than in the previous one (r = 0.981; p < 0.01). The difference between the two matrices mainly exhibits the huge effect in 2003, and to a smaller extent the developments in 1997, that is, the emergence of a new cluster of communication studies journals. However, the earlier change was crucial. In other words, the partial correlation coefficients provide descriptive statistics of the events visible in the animations. However, these measures cannot provide a measure of the three-way interaction effects.



**Figure 8**: The configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R = I - Q in millibits of information for the case of communication studies.

	Q	I <sub>ABC→AB:AC:BC</sub>	R	N
1994	-14	33	47	122
1995	69	52	-17	123
1996	51	34	-16	128
1997	67	81	14	139
1998	126	125	-1	144
1999	54	90	37	148
2000	70	88	18	149
2001	99	82	-17	155
2002	97	55	-41	158
2003	60	37	-23	162
2004	126	103	-22	157
2005	44	50	6	164
2006	81	50	-30	168
2007	94	80	-14	177

**Table 2**: The configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R = I - Q in millibits of information for the case of communication studies.

Figure 8 shows the development of the configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R = I - Q in millibits

of information. Table 2 provides this data in tabular format. The figure indicates the reorganization during the second half of the 1990s. Both curves peak in 1998 and 2004. 

The latter peak represents the recovery after the disappearance of the emerging configuration in 2003, and the former the initial emergence of communication studies as a structural component in 1998. This years corresponds with the spanning of a triangular structure among the three factors in the animation at <a href="http://www.leydesdorff.net/eigenvectors/commstudies">http://www.leydesdorff.net/eigenvectors/commstudies</a>. Appearing as an independent (third) factor for the first time in 1997, the component representing *Communication* 

Studies further develops into a separate dimension of the data in 1998.

On the basis of factor analysis in six dimensions, Leydesdorff & Probst (2009) noted the

further development of a group of journals about *Discourse Analysis* in 2006 and 2007. While the redundancy ( $\blacktriangle$ ) becomes decreasingly negative in the period 2002-2005, indicating that the configuration increasingly self-organizes the differentiation in terms of an intellectual organization, the volatility increases again thereafter. Perhaps one could expect a higher redundancy (R) in more stable fields of science, and this may lead to larger differences between I and Q. In these two case studies, however, the focus was on rearrangements in the structures and how these are indicated by Q and I. It seems that both Q and I can be used because the two indicators are correlated in the case of changes at the systems level. In this case, R does not play a significant role while the generation of uncertainty in the historical development is larger. How might this be different in the case of a relatively stable configuration?

<sup>&</sup>lt;sup>9</sup> The Pearson correlation coefficient between Q and  $I_{ABC \to AB:AC:BC}$  is 0.704 (N = 14; p < 0.05).

## c. The citation impact environment of the JACS

The citation impact environment of the *Journal of the American Chemical Society (JACS*) can be considered as such a stable configuration (Leydesdorff, 1991). This flagship journal of the American Chemical Society was founded in 1879 and had an impact factor of 7.885 in 2007. Its mere volume of approximately 3,000 publications each year makes the leading journal in the field of chemistry in terms of citations and references. In 2007, the citation impact environment of this journal consists of a structure of three main components, explaining 72.3% of the variance, and two smaller components which load on a fourth factor (explaining another 6.9%) with opposite signs. Table 3 provides the rotated component matrix for the four-factor solution of the journal-journal citation matrix.

	Component			
	1	2	3	4
Tetrahedron	.944			
Tetrahedron Lett	.941			
J Org Chem	.936	.197	106	
Eur J Org Chem	.922	.187	112	
Org Lett	.888	.301	121	
J Am Chem Soc		.889		.219
Chem-Eur J	.138	.881	.245	
Chem Rev	.295	.846		.265
Angew Chem Int Edit	.123	.769		203
Chem Commun	.212	.753	.426	261
J Organomet Chem	132		.845	
Dalton T	406	.230	.803	103
Organometallics	213	.118	.787	
Inorg Chem	400	.406	.572	
J Phys Chem A	190		139	.921
J Phys Chem B	494	.104	579	.334
Langmuir	448		576	218
Macromolecules	354	265	396	335

Extraction Method: Principal Component Analysis. Rotation Method: Varimax with Kaiser Normalization.

Rotation converged in 6 iterations.

**Table 3**: Four-factor solution for the citation impact environment of *JACS* in 2007.

The three major components (organic, general, and inorganic chemistry) are present in each year of *JACS*'s citation environment as the first three components, although in some years the order among them changes. In previous studies, these environments were studied both in terms of subject headings in the catalogue of the Library of Congress for validation purposes (Leydesdorff & Bensman, 2006) and in terms of their dynamic development (Leydesdorff, 1991). In sum, these three categories provide us with a relatively stable configuration of structural components.

The stability of the configuration can be illustrated with an animation using 

PajekToSVGAnim. 10 (This animation is available at 

<a href="http://www.leydesdorff.net/eigenvectors/jacs.htm">http://www.leydesdorff.net/eigenvectors/jacs.htm</a>. 11) It shows the extreme stability of the 
three-factor solution in terms of eigenvectors representing organic, general, and inorganic 
chemistry journals.

	Q	<i>I(ABC→AB:AC:BC)</i>	R	Ν
1994	-1014.1	0.1	1014.2	16
1995	-697.6	0.1	697.7	15
1996	-1210.7	0.1	1210.7	16
1997	-344.8	0.1	344.8	17
1998	-429.5	0.2	429.7	20
1999	-787.5	0.1	787.5	19
2000	-811.3	0.0	811.3	21
2001	-766.9	0.1	767.0	19
2002	-1201.9	0.0	1201.9	19
2003	-1177.2	0.1	1177.3	20
2004	-839.8	0.1	839.8	21

<sup>10</sup> PajekToSVGAnim.exe is freely available for non-commercial usage at <a href="http://vlado.fmf.uni-lj.si/pub/networks/pajek/SVGanim/default.htm">http://vlado.fmf.uni-lj.si/pub/networks/pajek/SVGanim/default.htm</a>. Unlike *Visone* this program allows for including negative factor loadings.

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<sup>&</sup>lt;sup>11</sup> Since SVG animations are not supported in Firefox, a streamed version of this animation (using flash) is also available at <a href="http://www.leydesdorff.net/eigenvectors/jacs/index.htm">http://www.leydesdorff.net/eigenvectors/jacs/index.htm</a>.

2005	-890.2	0.0	890.2	18
2006	-1182.7	0.0	1182.7	19
2007	-664.7	0.1	664.8	18
			$\overline{R} = 858 \pm 277$	

**Table 4**: The configurational information Q, Krippendorff's (2009a) ternary information term  $I_{ABC \to AB:AC:BC}$ , and the difference R = I - Q in millibits of information for the citation impact environment of JACS, 1994-2007.

Table 4 teaches us that  $I_{ABC \to AB:AC:BC}$  in this case is orders of magnitude smaller than R. In 1998, a maximum of 0.2 millibits of information is generated historically while the intellectual organization at the above-journal level reduces uncertainty by 430 millibits. The average reduction of uncertainty is 858 ( $\pm$  277) millibits of information.

Note that the values of Q are negative in all years. This means that the citation patterns among the three journal structures pervade one another in a configuration like that depicted schematically in Figure 2a (above). In summary, the (sub-)fields of chemistry do not develop in terms of their textual structures, but substantively at a level above the observable relations. This intellectual organization structures the components in the textual interactions; the observable history of the textual system does not generate uncertainty which cannot be absorbed by the configuration in the knowledge base of the system.

#### Conclusions and discussion

The results in the two cases of interdisciplinary developments suggest that both  $I_{ABC \to AB:AC:BC}$  and Q provide us with indicators of change in configurations among structural dimensions. Conceptually, however, the two measures are very differently

defined. Whereas  $I_{ABC \to AB:AC:BC}$  indicates Shannon-type information caused by the three-way interaction, Q is the difference between this historical uncertainty and the redundancy provided by the model. Since the model provides meaning to the historical events, one could also consider Q as a measure of meaningful information, that is, the difference between (Shannon-type) information and its meaning for a receiving system (e.g., an observer).

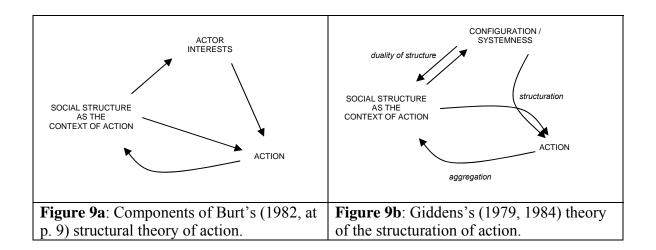
In the third case of stable disciplinary development, Q was strongly negative and the historical interaction among the components ( $I_{ABC \rightarrow AB:AC:BC}$ ) almost vanished. In this case, the observable network relations did not affect the interactions among the three components historically, but the information remained reflexively meaningful for the reproduction of the system as a knowledge-based configuration. Since I and Q are both high in the case of interdisciplinary developments (Figures 4 and 6), not only was uncertainty produced within the system, but this information was also meaningful at the systems level. In such configurations, the redundancy provided by the (self-organizing) model at the field level is used completely for the transmission of information. One could hypothesize that when the historical uncertainty (I) is larger than the redundancy provided by the knowledge base of the system—the model—is under pressure to reorganize. The addition of new categories, for example, would change the maximum entropy of the model.

(Partial) correlation coefficients among the structural dimensions provided us with descriptive statistics of changes. The latter could also be visualized by positioning the eigenvectors among the variables, that is, by using the rotated factor matrices as input to the animations. Insofar as one can observe an increase (or decrease) in complexity by using these animations, this has to be considered as Shannon entropy, since Q provides a difference which cannot be observed directly. The value of Q is an effect of the configuration which provides us with an algorithmic access (Equation 1) to the model generating redundancy. This model can be entertained by an external observer in the case of first-order cybernetics or an observing subroutine of the system. In the latter case, the theoretical frame of reference can be provided by the theories of both anticipatory systems (Rosen, 1985) and *autopoiesis* (Maturana & Varela, 1980; cf. Leydesdorff, 2009).

In other words, a model is offered for how knowledge can be generated and selforganized in networks. Beyond being generated, discursive knowledge can again be
communicated in the knowledge networks of social systems. Thus, the next-order level
loops back into the information processing (Maturana, 2000). The order of expectations
coevolves with the order of events in a knowledge-based system. The reflexivity of
human agency drives the loop because the expectations have to be articulated into new
knowledge claims. The distribution and communication of the latter provide the variation
on which the different selection mechanisms can operate. Note that the development of
discursive knowledge presumes the flexibilities of human language and reflexivity
(Giddens, 1984; Leydesdorff, 2000; Luhmann 2002b). Both recursions (with the arrow of
time) and incursions (against the arrow of time) are involved (Dubois, 1998).

Our model captures Giddens's (1979) concept of "structuration" and provides it with an empirical operationalization. Furthermore, this concept could be positioned with reference to Luhmann's (1995) social systems theory and Maturana and Varela's (1980) theory of *autopoiesis*. The mechanism for reproduction of structure in networks is different from—orthogonal to—the network structure itself. Structure is static and (re)produced at each moment of time. Giddens's dictum that "structure only exists as 'structural properties'" accords with the factor-analytic model: eigenvectors can be considered as structural components of a network.

The configuration among the hypothesized dimensions can be entertained as a model of structure by a knowledge-based system. Because the model is only available reflexively (that is, in terms of expectations), structuration should not be reified: it operates as a "duality of structure" but in a virtual domain (Giddens, 1979, pp. 81 ff.). This duality could be specified in terms of Shannon-type information aggregated into structure *versus* the redundancy generated by the model. *Q* measures the difference between these counteracting dynamics, that is, the imprint of the (self-)organization at the systemic level on the historical development of structures. The structural components or eigenvectors provide the historical instantiations of structure.



In Figure 9, a comparison between Burt's (1982) structural theory of action and Giddens's (1979, 1984) theory of structuration of action from Leydesdorff (1993, at pp. 50 ff.) is further elaborated. In the right-hand figure, Giddens's terminology is added to the arrows and the model changed in accordance with the three-layered model specified in this study (Figure 1 above). Systemness, however, should in this case be understood not in Giddens's (1979, at p. 66) sense as "reproduced relations," but as Luhmann's (and Husserl's) "horizons of meaning" which can be codified as universes of possible communications.

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