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# EVALUATING THE SCIENCE-TECHNOLOGY INTERACTION IN NANOTECHNOLOGY: A SIMULATION-BASED STUDY

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## ABSTRACT

Nanotechnology as an emerging, science-driven and rapidly evolving field with the multidisciplinary nature is an example of cases where science and technology are proximate and their interaction is essential. The scientific and technological networks can be formed separately in a social context and the linkages from the scientific to the technological network can be established through authors-inventors who act as gatekeepers and bridge the knowledge between the two communities. This work concerns individual researchers who are doing both, patenting and publishing, in the field of nanotechnology in Quebec Canada. An agent-based model was developed using real data regarding both nano-related articles and their authors, and nano-related patents and their inventors were collected from SCOPUS and USPTO databases respectively. While the repetitiveness in collaborative relationships has shown an enhancement in author-inventors performance, it negatively affects the knowledge flow efficiency. Author-inventors are fundamentals for increasing the network productivity and assure its interconnectivity.

## 1 INTRODUCTION

### 1.1 The Science-Technology Interface

Science and technology have been seen as 'dancing partners' that are closely connecting, time interacting yet interdependent systems. Academics and policy makers are getting more interest in understanding the complex relationship between science and technology at both regional and national levels. Several studies in the literature used different observational indicators to measure the increasing interdependencies and interactions between science and technology using different interpretations. These indicators are based on citations to non-patent literature, scientific publications from industry, co-authorship relationships between industrial and academic researchers, patents owned by academic institutions, patents invented by academic researchers but owned by industry and author–inventor links (e.g. Moed et al. 2004; Meyer 2006a; Cassiman et al. 2007).

In recent years, the growing studies have focused on investigating the impacts of academic patenting on the future scientific research. Although the understanding of the effects of university patenting on scientific research remains open to debate theoretically, a large body of empirical studies evaluating statistically the relationship between patenting and publishing have provided strong evidence that there is no negative effect of patenting activities on publication output of individual academic scientists, especially for star scientists (Meyer 2002; 2006a; 2006b). The results showed that patenting faculty members apparently outperform their non-patenting peers in terms of both quantity and quality of publication in the field of nanotechnology and the most productive scientists are those most likely to invent too and become author-inventors.

Author–inventors links in particular have been analyzed first in small scale studies, since the late 1980s and early 1990s (Noyons et al. 1994; Meyer 2006a) and then by compiling larger data sets matching inventor names with scientific author names, and by collecting data on individual researchers' patenting and publication performance (e.g. Boyack and Klavans 2008; Breschi and Catalini 2010; Wang and Guan 2011; Maraut and Martı´nez 2014).These studies characterized the relation between science and technology by the author-inventor links created by researchers who are co-active in publishing and patenting using matching and disambiguation techniques to create unique person identifiers in patent and publication databases (Lissoni et al. 2008; Raffo and Lhuillery 2009; Dornbusch et al. 2013). Author-inventors are the most productive and highly cited researchers, and have been identified as key individuals in the process of knowledge transfer. The science-technology conversion is also accelerated through author-inventors implement the conceptual principle of dual awareness (Kostoff 1997).

### 1.2 Networks of Collaborative Activities

The network of individuals can be created based on various kinds of social and collaborative relationships. The activities of collaborators and their partners can be mapped with a complex net, where several actors are represented as nodes (or vertices or agents), the linkages represent their collaborative relations and a new knowledge is the product of interplay between them. In case of the innovation networks, it is the individual researchers, or inventors, who are the network nodes. The analysis of co-authorship of research articles and the co-inventorship of scientific patents are the most commonly used methods employed to trace the linkages between these nodes, i.e. partners co-creating knowledge or innovation. The connecting link between two scientists in the network is created if at least one paper has been coauthored by them (Newman 2001; Barabási et al. 2002; Boccaletti et al. 2006) or if they have co-invented a patent together (Fleming and Frenken 2007).

Some studies examine the properties of networks at the nodes' level exploring the authorship relationships. The social network analysis (SNA) measures (i.e. normalized closeness centrality, normalized betweenness centrality, efficiency, degree and weighted degree centrality for each node) have been used to understand how the position of a collaborator at the network correlates to their research performance (Abbasi and Altmann 2011; Abbasi et al. 2012; Kas et al. 2012; Zamzami 2014). Other scholars examined the properties of co-invention networks exploiting the information contained in patent data. The main result of these studies showed the essential role of such social collaborative activities in knowledge diffusion represented be patent citations (Breschi and Lissoni 2005). Following this result, the network statistics have been used to identify the central player in patenting activities and how is their transmission affects the performance of isolated subnetworks (Fleming and Frenken 2007).

Combining both co-authorship and co-inventorship data together is a new approach introduced later by some scholars in order to investigate the link between the two communities considering their engagement in a wide range of activities, such as advising, consulting, licensing and establishing new firms (Murray 2002). Following this approach, some studies examined the relationship between patents and publications based on the analysis of publishing-patenting scientists (Meyer 2006; Boyack and Klavans 2008). The results showed that although the scientific and technological networks remain distinctive there is a slight overlapping between them. This overlap between the scientific and technological research networks has been investigated further by combining co-authorship and co-invention data and use social network analysis (SNA) (Breschi and Catalini 2010; Wang and Guan 2011). They used the author-inventors structural positions to identify their role in transferring the knowledge between the scientific and technological spheres and facilitate their interactions.

# 2 METHODOLOGY

## 2.1 Field of Study and Data Source

This paper presents the results of a dynamic study of the interaction between nano-technology and nano-science which are perceived as relatively closely related fields of science and technology. The study concerns the role of individuals who are active in both communities in Canada (Quebec). Nanotechnology innovation system has been identified as a dynamic process, involving multiple interacting and co-operating actors, variations of essential technologies, society and business models (Carlsson et al. 2002). The main data collection approach consists of the exploitation of extensive data about authors, inventors, as well as their performance and collaboration activities history. Based on the comparison of different digital libraries and online databases, SCOPUS for publications and USPTO for innovations (patents) have been found as the most suitable ones for this research purpose (Moazami et al. 2015). The complete database contains around 748,251 nanotechnology articles and 240,000 patents as well as the authors and inventors data including the city and province of the organization they affiliated to. We restrict our data set to the case where at least one of the co-authors is from Canadian organization located in the province of Quebec and at least one of the co-inventors with a residence in Quebec.

## 2.2 Matching Criteria

The approach is based on the matching of authors information from scientific publications with inventors information from patent filings in Canada-Quebec. The matching criteria have been considered to identify the common researchers from the two databases include the country of origin, the organization, name, location and ID. However, the matching process was a challenging considering that individuals have different name format in authors database than the one(s) in inventors database. The inventors information is complete, because patents are legal documents. However, the same inventor may register different patents under different formats of their name. For example; the inventor may register a patent with his full fist name, an initial of the middle name and the surname and can found in another patent with different format as full first name, full middle name and the surname. For Scopus on the other hand, from 1996 onwards, the large majority of authors' names containing the author's first name where there are few names with only an initial for the first name. The unification of names takes place across the databases by combining the selection criteria that are available in both.

Moreover, after combining the two data sets we have to analyze their overlap by identifying researchers who are found in both databases (author-inventors). In this respect, we have to deal with a major problem that is a scientist has different IDs in both databases. Thus, when we combine the two data sets the same person, who appears in both, will be considered as two different researchers. Further, it is difficult to perform a matching procedure based on the name format in the SCOPUS as it is most likely be registered with different format(s) in USPTO. To solve this, we used the previously mentioned matching criteria to match publishing-patenting scientists manually and unified their IDs using the one in SCOPUS.

## 2.3 Social Network Analysis

### 2.3.1 Approach for Constructing the Scientific-Technological Network

The collected data about authors (and their publications) and inventors (and their patents) will be combined and studied in social network context. We assumed that the nodes represent the individual scientists and their collaboration in patenting and/or publishing activities form the edges (links).

The first step to construct this network is creating the scientific and technological linkages based on the extracted data regarding the collaboration activities between co-authors and co-inventors respectively. Second, the link between the two networks will be established through the identified common researchers who are participating in publishing an article and patenting an invention. We can classify the researchers (nodes) in the combined network into three categories: only-authors (i.e. researchers that participate in the co-authorship network only), only-inventors (i.e. researchers that participate in the co-invention network only) and author-inventors (i.e. researchers active in both networks).

The figure below illustrates an example of the combined network idea which is a hypothetical network of 17 scientific authors, 13 inventors and 3 author-inventors, identified respectively by the suffixes A, I and AI. The network consists of two layers. The authors of scientific publications and co-authorship relationships form the top layer while the inventors of patents and their links, form the bottom one. Author-inventors work as gatekeepers who are responsible for the connectivity between the two layers (the scientific and technological networks) (Breschi and Catalini 2010).

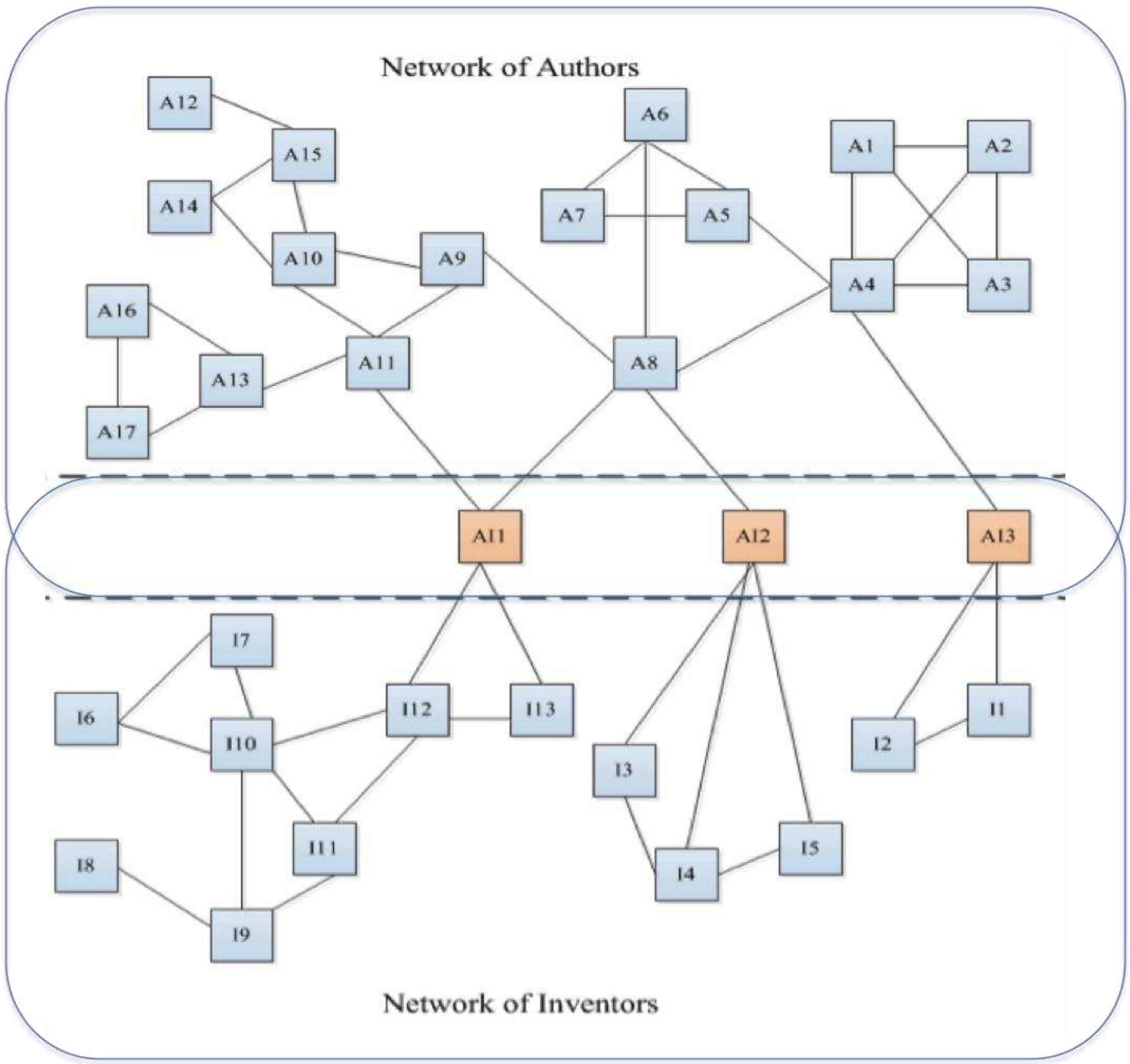


Figure 1: A hypothetical network of inventors and scientific authors.

### 2.3.2 Measuring the Mathematical Properties of the Network

The scientific-technological network mathematical analysis includes evaluating its structure based on some measures calculated by applying the graph theory. The following indicators for the whole network and each node (representing a researcher in our network) will be measured:

- **Network Density:** The network density as defined by de Noyons, et al. (2005) is the percentage of actual lines present in the network to the maximum possible number of arcs and it depends on the size of the network. The higher density indicates higher number of connections among the nodes, more interaction between the scientists, leading to a tighter structure and a more cohesive network.
- **Betweenness Centrality:** An actor's potential control of communication within the network can be indicated by betweenness centrality (Chung and Hossain 2009; Abbasi and Altmann 2011). It is defined as the ratio of the number of shortest paths (between all pairs of nodes) that pass through a given node divided by the total number of shortest paths. The highest betweenness centrality suggests the most central vertices. In other words, vertices (researchers) with high betweenness centrality play critical role in bridging the knowledge between different nodes that are directly connected to the most central ones. Some scholars hypothesize that, researchers who act as bridges in the cooperative network have more control and are more productive (Breschi and Catalini 2010; Zamzami 2014).
- **Degree Centrality:** Degree centrality is an indicator of an actor's communication activity (Chung and Hossain 2009; Abbasi and Altmann 2011). In a simple undirected network the degree of a vertex specifies the number of its neighbors. Likewise, the degree of each vertex, which represents a researcher, indicates how many collaborators he/she used to work with.
- **Clustering Coefficient:** The clustering coefficient (CC) of a vertex (node) in a network graph quantifies how close its neighbors are to being a clique (complete graph). In other words, it shows how related each researcher is to his/her neighbors at the same community, and the probability that they become a closed research group. Clustering coefficient is simply the number of edges between the neighbors, divided by the maximum possible for the type of network, $k\ (k\ -1)$ or $k\ (k-1)=\ 2$. It is worth mentioning that the clustering coefficient is decreasing over the years, with around 20% chance of two scientist collaborating if both have done so with a third scientists (Perc 2010).

### 2.4 The Simulation Approach

We conduct experiments in computer-generated scientific-technological network, and simulate the collaborative behavior of inventors, authors and author-inventors researchers. The experiments are implemented using Netlogo (v. 5.0.4), a multi-agent programmable modeling environment (Wilensky 1999). The basic units of our proposed model are a set of agents or nodes representing the researchers, where two nodes are connected by a link if these two individuals have collaborated in a publication, patent or both. Several scenarios, such as the presence, absence and repetitive collaboration, are simulated in order to determine the impact of some changes on the network structure and researchers scientific and technological production.

#### 2.4.1 Building the Conceptual Model

An extensive analysis of the real world has been conducted in order to build the conceptual model and be able to set some assumptions. The maximum number of potential partners, for example, has been determined referring to the degree probability analysis of the database. Based on the probability density function, we have found that the highest likelihood is to have no more than 10 partners. Accordingly, we have assigned 10 as the maximum allowable candidates that an author will search for, while each will have an actual partnership with the preferable number the model learned from the collaboration history.

Moreover, the patenting share percentage for each time unit has been assigned to 0.33 based on different factors. First, the average duration of the registration process at USPTO for a patent to be granted is 3 years. The other factor is the proportion of the patents to the articles by author-inventors identified in our database, which is almost 0.3. Furthermore, giving the change rate in the publications and patents volume over the study period, the model representing the evolving trend by increasing the number of starters by a random percentage between 1.34 and 2.54 every year, thus the outcome will be increased by a ratio corresponding to reality.

### 2.4.2 General Model Description

Our preliminary results are based on around 5,700 researchers including Quebec-based authors, inventors, author-inventors and their partners. We constrain the environment to be closed: no new researchers will join the network at the moment. There are few assumptions that agent will share regarding the collaborative behavior including the preferred partner and percentage of researchers initiates the partnership as explained above.

There are two phases to each model SETUP and GO. In the SETUP phase, the initial values for set of agents' parameters will be loaded into the model through reading text files created based on proper SQL queries from our database. The second text file contains information about the collaborative activities history. It consists of the co-authorship relationships between each two scientists that will be represented as links in our model. All scientists who have prior collaboration with a researcher will be stored as his/her previous-partners agent set. Considering that this is a two-way relationship, the pair of scientists at both ends of each link will be added to be referred to while seeking partners for new collaboration. In the GO phase, the model will assign a random number of nodes that will be acting as starters who will initiate the partnership process by searching for candidates to collaborate with. An agent can be involved in more than one collaboration activity at the same time with a maximum number of partners for each involvement.

Based on the real world analysis, a potential partner who has a satisfactory prior collaboration experience with an author will most likely attract him/her for a new one. This is reflected in the model by the repeated collaboration function: to find a partner, a starter will seek among previous partners agent set and assign some as candidates. The number of candidates should not exceed the maximum allowable number of partners. The most centralized nodes, (i.e. gatekeepers, nodes with highest betweenness) will be also attractive to be selected as candidates for new collaborations and will be most frequently selected over others to act as potential partners. In fact, several factors were considered for forming the collaboration tie within the model based on the results of a survey was previously conducted in order to improve our understanding of the partners' selection mechanism. Questionnaire was sent to the previously identified active researchers in our database who have a scientific collaboration history. The findings show that the most critical factors to be considered while selecting the partners are: their academic reputation, their experience in a complementary field, the resources and funding accessibility, the previous collaboration relation with them and its strength (Zamzami 2014).

After finding the candidates, the partnership relationship will be established, where for some of them it will be based on the preferable number of partners according to past collaboration. If this is the first time for a pair of scientists to collaborate a new link will be created between them and a value of 1 will be given to its strength. Alternatively, if the collaboration tie between them already exists, its strength will be incremented by 1. That is, 0.5 for each side of the relationship to avoid the redundancy.

Each researcher in the model (node) is in one of three categories: author, inventor and author-inventor. We are assuming that each collaboration activity is resulting in a new publication (for authors), a participation in a patent (for inventors) and both for the author-inventors. Thus the variable (Nano articles) for agents involved in each network will be increased by 1 where (patents) will increase by 0.33. Besides, the actual partners will be added to previous partners agent set for a future collaboration that might occur in the next iterations.

Only agents that have participated in any collaboration activity during this step (iteration) will be given an age value equal to the step number x. These agents will form the new network whose structure and productivity will be examined. For all nodes with (age = x) we will recalculate the values of variables related to network measurements. The Netlogo NW extension for network analysis have been integrated with our model to reanalyze the network in each iteration based on the new collaboration activities. The degree centrality, betweenness centrality and clustering coefficient for each node in the new network will be updated as values for the associated variables. After updating the values the structure measurements for the whole network will be calculated by averaging the values of individual participants. The flowchart below describes the sequence of the process in the developed model.

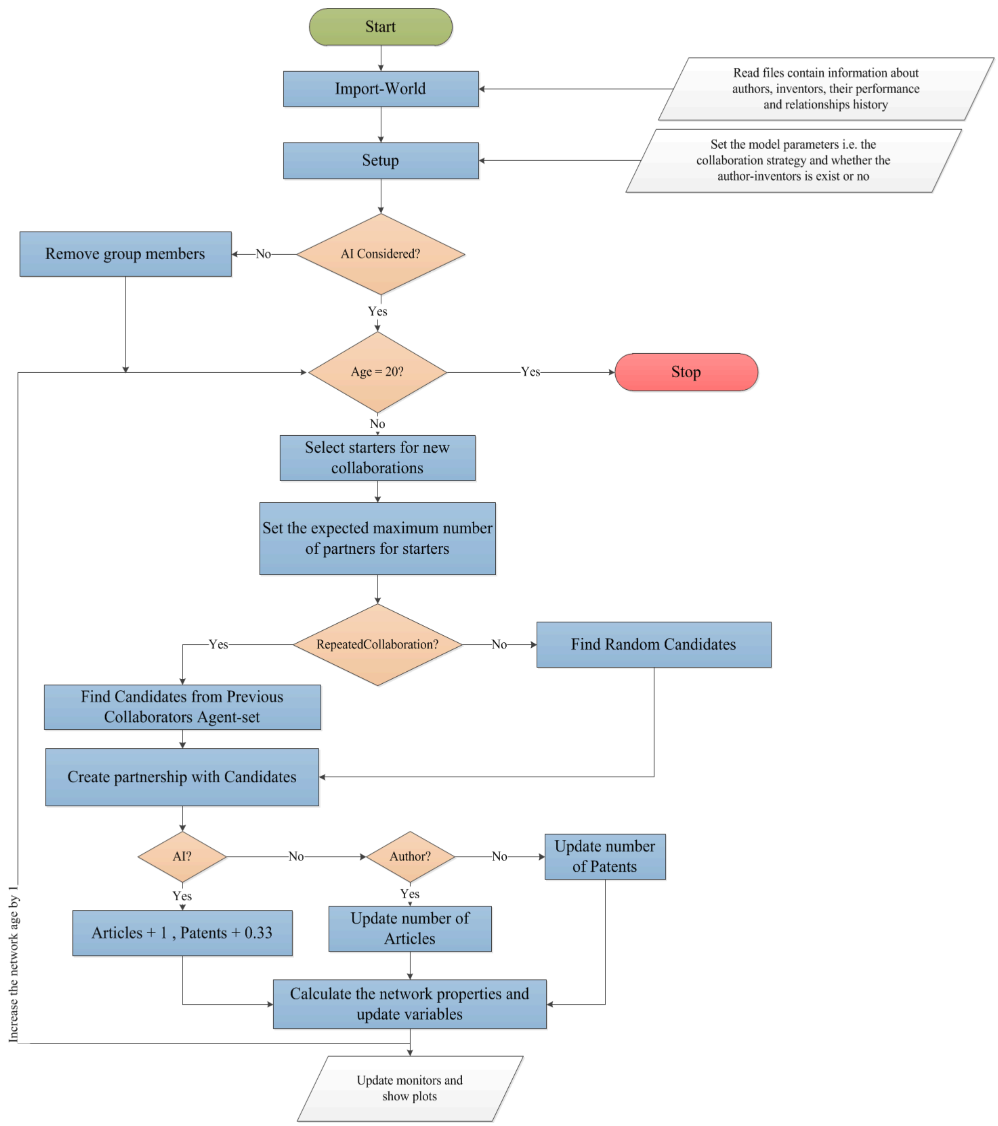


Figure 2: Flowchart of the developed simulation model.

The original setting will be used for running the default situation of the model. We ran several scenarios including changes in real world parameters to study the role of author-inventors and the impact of their loyalty on the network performance and structure.

## 3 SIMULATION AND EMPIRICAL RESULTS

Indeed, the author-inventors are parts of the scientific-technological network, that is, they appear and grow in the network naturally. Accordingly, the hypotheses regarding their behavior as well as their absence from the network can by justified only through simulated scenarios and not by real evidences. To examine the impact of the absence of this group on the production and the structure of the network, a substitution for the real world would be required.

The parameter variability analysis is implemented by carrying out several experiments to examine the effect of changing the values of the input and internal parameters of the model upon the model's behavior or output. Various scenarios are simulated to study the role of author-inventors first by changing their collaboration behavior and then by removing them completely from the network.

Using BehaviorSpace, a software tool integrated with NetLogo that allows you to perform experiments with models, we have run the model many times, systematically varying the model's settings "parameter sweeping" and recording the results of each model run. Beside the basic scenario where author-inventors are most likely repeating their successful partnership, the experimental scenarios used different values for the chooser reflecting the collaboration strategy (repeated collaboration, new collaboration). The objective of this set of scenarios is evaluate the impact for the author-inventors' loyalty on the overall productivity and network structure.

The other experimental scenarios used two values for the switch (true and false) reflecting the existence and absence of this group respectively. The objective of these scenarios is to examine the role of author-inventors by removing them completely from the network. In other words, in the other scenario we have removed author-inventors along with their links (i.e. their collaboration ties will be removed also, but their partners will remain in the network open for new partnerships).

In each scenario, we have used 10 replications of each experiment, and the results are then averaged for these ten runs of the model. We have examined the change of one value only while the rest of the settings remain the same. For comparing and evaluating the scenarios we are mainly concerned about the performance and the structure of the network.

As for the performance, the number of publications and patents for the whole network and the average of the articles published and patents invented by the author-inventors group are used as indicator of the productivity. On the other hand, we have examined the structure of the network as it plays the key role in the diffusion of knowledge and production of innovation. The network structure properties have been calculated by averaging the values of the corresponding variables for all nodes that the network consists of. Degree centrality, betweenness centrality, clustering coefficient and network density have been calculated and compared in the different scenarios to evaluate the impact of the changed setting.

### 3.1 The Impact of Loyalty on the Scientific-Technological Network

The first series of scenarios examines the effect of the repetitiveness of the collaborative relationships on the network overall scientific and technological productivity and its knowledge transmission capability. The scientists are more likely to repeat their successful partnerships and thus be loyal to their own partners. In the model, around 60% of the starters will first search for partners among their partnership agent set (to whom they collaborated before). By changing the probability of old partners to be selected again, the loyalty will be decreased and new nodes will get a chance to access a new knowledge source. To compare the various scenarios, the network properties were measured and analyzed.

The simulation experiment has been run for 20 (time units) for each collaboration strategy (repeated collaboration, new collaboration). The results showed that the average productivity of author-inventors enhances as their social ties become stronger in the network. However, others especially those who are new to the firm will probably lose their chance to collaborate and thus their performance declines. Moreover, the results showed that repetitive collaborative relationships affects the structure of the innovation networks negatively, resulting in more cliquishness and less knowledge transmission among agents of the network reflected by the higher average clustering coefficient and lower average betweenness centrality respectively (See Table 1 below).

With new collaboration relationships, the researchers will have more chances to gain external knowledge instead of being limited within a closed research group or community.

Table 1: Simulation results for the impact of loyalty.

| Collaboration Strategy | Ave. Betweenness Centrality | Ave. Degree Centrality | Ave. Density | Ave. Clustering Coefficient |
|---|---|---|---|---|
| Repeated Collaboration | 0.0184 | 6.196 | 1.278 | 0.498 |
| New Collaboration | 0.0205 | 6.289 | 1.357 | 0.430 |

### 3.2 The Role of Author-inventors in the Innovation Network

The next two scenarios relate to the role of author-inventors in the connectivity, knowledge generation and transmission among the scientific and technological communities. This has been examined through the comparison of the effects of their presence and their absence on the overall productivity and structure of the networks.

To run the scenario of their absence, the nodes representing author-inventors will be asked to "die" (the node will be removed completely from the world along with the collaborative links they entertained). The mathematical indicators of the scientific-technological network are then analyzed and compared for both scenarios, with and without the author-inventors.

The simulation experiments have shown that both, total number of publications and patents, are higher when author-inventors are included. The presence of author-inventors therefore, has a positive impact on both scientific and technological productivity of the network. The overall network characteristics are comparable for the two scenarios.

As the density is related to the size of the network, the removal of some nodes (author-inventors) would let to a smaller network size. However, due to the small percentage of this category comparing to the population (about 2.89%) the change in this measure for the both scenarios is relatively inconsiderable. However, the existing of author-inventors is critical to assure more interconnectivity (higher average betweenness centrality) and consequently better flow of knowledge among authors and inventors, which would result in faster transmission of knowledge in the network. The table below summarizes the network measures in the two scenarios.

Table 2: Simulation results for the role of author-inventors.

| Scenario | Ave. Betweenness Centrality | Ave. Degree Centrality | Ave. Density | Ave. Clustering Coefficient |
|---|---|---|---|---|
| Author-inventors included | 0.0184 | 6.196 | 1.278 | 0.498 |
| Author-inventors excluded | 0.0171 | 6.194 | 1.261 | 0.483 |

## 4 CONCLUSION

The developed simulation model is the first one to implement combining co-authors and co-inventors data, and the analysis of publishing- patenting scientists approaches in a dynamic context. It aims to evaluate the interaction between science and technology considering the knowledge flows and transmission within the scientific-technological network. Our concern is to study the network at individual level to investigate the role of author-inventors, who act as gatekeepers, and their collaborations in enhancing the innovative and research performance as well as the network efficiency. An agent-based simulation model of the authors and inventors was developed and the simulation experiments employed for various scenarios.

Although the loyal author-inventors showed a good scientific production, others scientists will have better performance in case they got higher probability to be selected as new partners. The results, on the other hand, suggest that loyalty, i.e. maintaining strong collaboration ties to previous partners, negatively affects the knowledge transmission capability of the scientific-technological network over time. That is, strongest collaboration ties would make the network more embedded and consequently degrade the knowledge transmission. As for author-inventors, we have proved their critical role in enriching both the scientific and technological production. Moreover, they are facilitating the knowledge exchange between the two communities and act as gatekeepers who are responsible for bringing new knowledge into otherwise closed and separated networks.

The contribution of this research is the essential first step towards studying the performance of scientific-technological networks in dynamic context. Many real-world problems were simplified or ignored due the need for more data or because their solutions were outside the scope of this research. We intended to use more comprehensive database(s) where more information about the field of expertise, research interests and funding amount each scientist receives could be collected to improve the partner‘s selection mechanism in the model and reduce the level of randomness. Another direction for future research, which is even more realistic, is to consider some details about the scientists' research career, i.e. change in their positions and/or mobility between different firms or organization. These changes might affect their productivity and open new opportunities for different type of partnerships.

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