The Emergence of Higher-Order Structure in Scientific and Technological Knowledge Networks*

Thomas Gebhart\textsuperscript{1} and Russell J. Funk\textsuperscript{2}

\textsuperscript{1}Computer Science and Engineering, University of Minnesota
\textsuperscript{2}Carlson School of Management, University of Minnesota

Abstract

The growth of science and technology is primarily a recombinative process, wherein new discoveries and inventions are generally built from prior knowledge. While the recent past has seen rapid growth in scientific and technological knowledge, relatively little is known about the manner in which science and technology develop and coalesce knowledge into larger structures that enable or constrain future breakthroughs. Network science has recently emerged as a framework for measuring the structure and dynamics of knowledge. While helpful, these existing approaches struggle to capture the global structural properties of the underlying networks, leading to conflicting observations about the nature of scientific and technological progress. We bridge this methodological gap using tools from algebraic topology to characterize the higher-order structure of knowledge networks in science and technology across scale. We observe rapid and varied growth in the high-dimensional structure in many fields of science and technology, and find this high-dimensional growth coincides with decline in lower-dimensional structure. This higher-order growth in knowledge networks has historically far outpaced the growth in scientific and technological collaboration networks. We also characterize the relationship between higher-order structure and the nature of the science and technology produced within these structural environments and find a positive relationship between the abstractness of language used within fields and increasing high-dimensional structure. We also find a robust relationship between high-dimensional structure and number of metrics for publication success, implying this high-dimensional structure may be linked to discovery and invention.

\*E-mail gebhart@umn.edu or rfunk@umn.edu. We thank the National Science Foundation for financial support of work related to this project (grants 1829168 and 1932596).
1 Introduction

The past 100 years have witnessed greater progress in science and technology than perhaps any other period in human history. Against this backdrop, many observers have expressed concerns over the possibility of science and technology becoming victims of their own success [Cowen and Southwood, 2019, Bloom et al., 2020]. As science and technology have grown, so too has the knowledge that researchers must master before arriving at the frontiers of their fields, thereby making future advances slower and more challenging [Jones, 2009, Milojević, 2015, Agrawal et al., 2016, Pan et al., 2018, Chu and Evans, 2018]. A different line of thinking suggests that future developments in science and technology are unlikely to measure up to the past, as many of the most important (and easiest) breakthroughs may have already been made [Arbesman, 2011, Cowen, 2011, Gordon, 2017]. While such concerns are not new—Einstein and others, for example, were already remarking on the burden of knowledge in the 1930s—there is growing empirical evidence of several seismic shifts in the social organization of science and technology that align with these views, including the move to team-based production [Wuchty et al., 2007, Wu et al., 2019], greater emphasis on interdisciplinary research [Leahey et al., 2017], and the changing structure of careers [Jones, 2010].

Recently, studies have devoted increasing attention to developing techniques for characterizing the structure and dynamics of scientific and technological knowledge. While true progress is difficult to measure (and even define), such characterizations are useful both because they enable more systematic ways of documenting change and for the potential clues they offer into the underlying mechanisms. To date, perhaps the most common approach in this literature has been to represent knowledge as a network—where nodes represent concepts, discoveries, or inventions, and edges represent relationships among them—and then to leverage techniques from network science to examine patterns of connection over time [Uzzi et al., 2013, Rzhetsky et al., 2015, Acemoglu et al., 2016, Christianson et al., 2020, Dworkin et al., 2019]. Conceptually, this approach is attractive because it maps well onto theories that suggest advances in science and technology result from recombinations of existing knowledge. [Schumpeter, 1983, Fleming, 2001] Findings using network approaches largely underscore prior observations of dramatic changes in the structure and dynamics of scientific and technological knowledge, but they also add important nuance. In addition to growing in volume, scientific and technological knowledge has also become more complex, as measured by the degree of interconnectedness among components [Shi et al., 2015, Varga, 2019]. Authors also observe that bridging—a common proxy for innovation, in which an idea spans two or more disconnected areas of a knowledge network—has declined precipitously over time [Mukherjee et al., 2016, Foster et al., 2015].

While existing network approaches have been helpful, they are also limited in several important respects. Most critically, they tend to focus on lower-level, dyadic interactions among knowledge components. Given the enormous volumes of prior scientific and technological knowledge, however, discovery today may be more like a game of high-dimensional chess, requiring different lenses for seeing significant moves for comprehending the state of play. Thus, the focus of existing approaches on lower level interactions may offer one explanation for observed slowdowns; progress in science and technology may be playing out in places where current tools are not looking. Indeed, such a possibility may further account for how it is possible to observe slowing progress on macro indicators simultaneously with announcements of seemingly major breakthroughs in many fields, including the measurement of gravity waves and advances in deep learning, among others.

In this study, we develop a framework for characterizing the higher order structure of knowledge in science and technology. Our method shares with prior work the notion of representing knowledge as a network, but differs in its analytical approach. We leverage methods from algebraic topology to characterize the meso- and macro-scale structure of technological and scientific knowledge, beyond pairwise interactions. We compute the persistent homology of these knowledge networks and observe the emergence of a dynamic landscape of high-dimensional structure across time that is not readily captured by traditional network-theoretical methods. We find that the structure of many fields of science and technology has seen a rapid rise in higher-order homology. Leveraging persistent homology, we are able to further characterize the structure of scientific and technological knowledge networks in terms of their knowledge co-occurrence frequency, providing a principled multi-scale comparison of knowledge structures both within and between fields. This multi-scale characterization reveals that the structure of knowledge is generally diverging between fields over time. We also find that this structural divergence is much more pronounced when comparing knowledge networks to the co-author collaboration networks that produce them, reinforcing the idea that the complexity of knowledge is outpacing the collaborative complexity of scientists and technologists. We find that the terminology used
Figure 1: Persistent homology of complex networks. A. Graphical representation of a knowledge (or collaboration) network. B. Transformation of the network into a flag complex. Nodes become 0-cells, edges become 1-cells, 3-cliques become 2-cells, etc. Homological features are denoted by circular and spherical voids. This flag complex contains a single connected component ($\beta_0 = 1$); two 1-dimensional, circular holes ($\beta_1 = 2$); two 2-dimensional, spherical holes ($\beta_2 = 2$); and no higher-dimensional holes ($\beta_3 = 0$). C. Filtration of the complex above varying inverse edge weight threshold $\epsilon$. Topological features in each dimension are tracked on the persistence diagram as $\epsilon$ increases. Here, the color of the points correspond to homological dimension. D. After all edges have been added in the filtration, points at infinity correspond to homological features that are never destroyed after they appear in the filtration. These points at infinity correspond to the Betti numbers (topological holes of a given dimension) of the simplicial complex.

within works situated in fields with high-dimensional structure tend to be more abstract than those situated in fields lacking high-dimensional structure. Finally, we observe a robust relationship between the existence of high-order structure in a field and a number of measures related to high-impact work. Taken together, these results suggest that the growth in productive scientific and technological knowledge is taking place at increasingly higher levels of structural complexity, with pairwise relations between granular knowledge areas as drivers of innovation being replaced by higher-order relations that represent more abstract knowledge. This growth in knowledge complexity necessitates tools like persistent homology that can formally characterize the movement between local knowledge and global high-order structure.

2 Methods

We begin this section by providing a brief overview of homology and persistent homology on networks. For a comprehensive overview of homology and its importance in algebraic topology, see Hatcher et al. [2002]. Additionally, Carlsson [2009] and Ghrist [2008] both serve as excellent introductions to the field of applied topology and the usage of persistent homology therein, and Aktas et al. [2019] provides a review of these tools applied to complex networks. We finish this section by providing a description of the data used in this study and its associated network structure.

2.1 Persistent Homology

Assume a weighted graph $G = (V, E, w)$ where $V$ is the set of vertices, $E$ the set of edges, and $w : E \to \mathbb{R}^+$ a function mapping edges to their weights. Let $w$ define an ordering on the edges of $G$ such that we may
decompose $G$ as a sequence of subgraphs $\varnothing = G_0 \subset G_1 \subset \cdots \subset G_M = G$ where $M$ is the number of distinct edge weights of $G$. Here $G_i$ is the subgraph of $G$ including only the edge(s) of highest weight. Each inclusion of $G_i$ into $G_{i+1}$ (i.e. $G_i \hookrightarrow G_{i+1}$) is the inclusion of the subgraph $G_i$ into the larger graph $G_{i+1}$ that includes all of $G_i$ and additional edges with weight equal to the $(i+1)$-th largest weight. At each step $i$ in this decomposition of the graph, we compute the clique complex or flag complex $K(G_i)$ of $G_i$ by treating each $k$-clique of $G_i$ as a $(k-1)$-dimensional simplex or cell. In other words, we “fill in” all cliques of the graph at each step $i$ such that 0-cells correspond to nodes, 1-cells to edges, 2-cells to 3-cliques (triangles), 3-cells to 4-cliques (tetrahedra), etc. More generally, each $k$-cell $\sigma = (v_0, v_1, \ldots, v_k)$ is the convex hull of $k + 1$ affinely-positioned nodes. We denote the set of $k$-cells $\Delta_k$. $K(G_i)$ is an abstract simplicial complex, meaning it is closed under taking subsets of $V$, so any subset of a cell must also be a cell. The filtration of $G$ extends to a filtration of simplicial complexes of $G$ such that $\varnothing = K(G_0) \hookrightarrow K(G_1) \hookrightarrow \ldots \hookrightarrow K(G_M) = K(G)$. See Figure 1 for an example of the construction of simplicial complexes from a graph (B) and the associated filtration (C).

We note briefly that this filtration and simplicial representation over $G$ is equivalent to the Vietoris-Rips filtration of the point cloud represented by $V$. To see this, consider the pairwise-distance between points $(u, v) \in E$ given by $\frac{1}{w(u,v)}$ such that points not connected in the graph have infinite distance. We can construct the Vietoris-Rips filtration from these distances and its homology will be identical [Ghrist, 2008].

To track the topological holes of $K(G_i)$, we introduce the chain group $C_k(K(G_i))$ which is a vector space with basis elements the $k$-cells of $K(G_i)$. Elements of $C_k(K(G_i))$ are linear combinations of these basis elements and are referred to as $k$-chains. We have freedom in the choice of coefficient field for this vector space with different choices offering different interpretations of the corresponding homology. We use $\mathbb{Z}_2$ in this work for computational simplicity and ease of interpretation.

To find holes in particular dimensions, we need to know how cells in higher dimensions map onto lower-dimensional cells. We define the boundary operator $\partial_k : C_k \to C_{k-1}$ as

$$\partial_k(\sigma) = \sum_{i=0}^{k} (-1)^i (v_1, v_2, \ldots, v_{i-1}, v_{i+1}, \ldots, v_k).$$

Note that applying the boundary twice yields zero, $\partial_k \circ \partial_{k+1} = 0$. Cycles in dimension $k$ correspond precisely to the elements of $C_k$ that are mapped to zero by $\partial_k$. In other words, the cycles of $C_k$ are elements of $\ker \partial_k$. The image of the $(k+1)$-dimensional boundary, $\im \partial_{k+1}$, comprise the $k$-boundaries. Intuitively, $\partial_{k+1}$ takes the interior of a $(k+1)$-dimensional simplex to its boundary. Therefore, $\im \partial_{k+1} \subseteq \ker \partial_k$ and $\partial_k \circ \partial_{k+1} = 0$ as expected.

But what about the elements of $\ker \partial_k$ that are not in the image of $\partial_{k+1}$? It is these elements that form the $k$-dimensional holes of the simplicial complex. We would like to count the number of $k$-dimensional holes within the simplicial complex, but there may be many cycles which, by the definition of $\partial$, form a boundary of this $k$-dimensional hole. As such, we must associate all cycles enclosing each unique $k$-dimensional hole. In other words, we form an equivalence class of the cycles by associating any two cycles $x, y \in \ker \partial_k$ if $x - y \in \im \partial_{k+1}$.

We now have the machinery necessary to define the homology groups of simplicial complexes. The homology group in dimension $k$ of simplicial complex $K(G)$ is precisely the group formed by the equivalence classes described above. Formally, $H_k(K(G)) = \ker \partial_k / \im \partial_{k+1}$. The rank of this group $\beta_k = |H_k(K(G))|$ corresponds to the number of $k$-dimensional holes in $K(G)$. We refer to the rank of this group as the $k$-th Betti number.

Recall that the inclusion relationship induced by edge weightings on the graph, $G_i \subset G_{i+1}$ extends to a filtration on the associated simplicial complexes $K(G_i) \hookrightarrow K(G_{i+1})$. This inclusion relationship over the simplicial structure extends also to the chain groups such that $C_k(K(G_i)) \hookrightarrow C_k(K(G_{i+1}))$ by mapping basis elements of $C_k(K(G_i))$ to basis elements of $C_k(K(G_{i+1}))$. Note that the homology of $K(G)$ is defined solely in terms of the chain groups. This implies that, for proper choice of basis, we can map cycles to cycles through the induced map $H_k(K(G_i)) \hookrightarrow H_k(K(G_{i+1}))$. Through this mapping on homology groups, we can track holes across the entire filtration of $G$. We refer to the point in the filtration at which a hole appears as its birth and the point at which it disappears its death. The difference between these quantities death - birth is called the lifetime of the hole. We can encode the global topology of $K(G)$ across its entire filtration conveniently as points in the upper-half plane known as a persistence diagram (Figure 1 C). Each point on
the persistence diagram in dimension \( k \) corresponds to a \( k \)-dimensional hole. Points near the diagonal may be considered “topological noise” as they represent holes with small lifetimes that are closed soon after they are born. In contrast, points located significantly the diagonal may be considered inherent topological features of the space as they appear early in the filtration and are closed late. Holes that never die over the course of the filtration correspond to points with death time at infinity which are the elements of \( H_k(K(G)) \). Their multiplicity is exactly \( \beta_k \).

The space of persistence diagrams is endowed with a natural distance metric. Given two persistence diagrams \( P_1 \) and \( P_2 \), we define a \( p \)-norm optimal transport distance as

\[
W_p(P_1, P_2) = \inf_{\phi: P_1 \to P_2} \left( \sum_{x \in P_1} \| x - \phi(x) \|_p \right)^{\frac{1}{p}}.
\]

For \( p = \infty \), Equation 1 is known as the bottleneck distance between \( P_1 \) and \( P_2 \). The bottleneck distance corresponds to the distance transported between the two farthest points under an optimal transport map. This distance is known to be stable to the underlying topology of the persistence diagrams such that small changes in the topology correspond to small changes in the bottleneck distance [Cohen-Steiner et al., 2007]. Another useful distance between persistence diagrams is the Wasserstein distance which corresponds to Equation 1 with \( p = 2 \). Although it does not enjoy the same stability guarantees, the Wasserstein distance is preferred to the bottleneck distance in our usage due to its increased expressiveness and intuitive \( \ell_2 \) averaging of the optimal transport map between points in \( P_1 \) and \( P_2 \).

### 2.2 Data Description

To characterize the higher-order network structure of knowledge in science and technology, we collected data from two large sources: (1) the American Physical Society corpus (hereafter “APS data”), consisting of more than 630,000 scientific articles published between 1893 and 2018, and (2) the U.S. Patent and Trademark Office’s (USPTO) Patents View database (hereafter “USPTO data”), which covers over 6.5 million patents granted by the USPTO from 1976 to 2017. For our purposes, both sources are useful for their well-developed knowledge categorization systems. The APS tags all published manuscripts in its corpus by subject with between 1 and 5 Physics and Astronomy Classification Scheme (PACS) codes (e.g., 04.30.-w, “Gravitational waves”; 14.60.Ef, “Muons”; 05.60.-k, “Transport processes”). PACS codes are hierarchical; at the most granular level, there are approximately 7,300 codes. Similar to the APS, the USPTO codes all patents by subject using between 1 and 99 classes drawn from its hierarchical, U.S. Patent Classification (USPC) system (e.g., 712/10+，“Array processors”, 558/486, “Nitroglycerin”; D13/165, “Photoelectric cell”). Relative to PACS codes, the USPC system is substantially larger, with more than 158,000 categories at the most granular level. The USPC system is regularly updated to account for changes in technology. With each update, the USPTO retrospectively reassigns (as necessary) the codes given to all previously granted patents. Thus, the USPC codes assigned to a particular patent may change over time.

We limit our focus to the period from 1980 to 2010 for papers and from 1976 to 2010 for patents. PACS codes were introduced in the mid-1970s, but they were not applied consistently in our data for the first few years. In addition, while the USPTO dates back to 1790, patent data are only readily available in machine readable form from 1976. Beginning in the mid-2010s, the APS and USPTO began retiring the PACS and USPC systems, respectively, in favor of new knowledge categorization systems. In addition, as we describe in more detail below, several of our analyses consider the implications of knowledge network topology for future discovery and innovation; as such, concluding our analyses in 2010 helps us to limit right censoring.

Following prior work, we limit our focus to utility patents, which encompass the vast majority (roughly 90 percent) of all patents granted by the USPTO. Thus, we exclude from our analysis design patents, plant patents, reissue patents, and several other smaller categories that are distinctive from utility patents in their nature and scope.

Even after limiting our focus to utility patents, the space of technologies encompassed by the USPTO data remains large and heterogeneous, spanning everything from furniture to semiconductors. We therefore characterize the knowledge network topology of the USPTO data separately for broad subfields of technology, using National Bureau of Economic Research (NBER) subcategories, of which there are 36 (e.g., “Biotechnology”, “Communications”). We occasionally present our results by aggregating to the level of the NBER
category, of which there are six (e.g., “Drugs & Medical”, “Computers & Communications”), and within which the subcategories are embedded. Because they primarily cover a single discipline (physics), we do not characterize the knowledge network topology of the APS data separately for subfields.

We also consider collaboration networks in some of our analyses. In collaboration networks, nodes correspond to authors; edges indicate co-authorship. When mapping instances of authorship to authors (our nodes), our data pose a challenge because neither patent inventors nor paper authors are assigned unique identifiers at the time of publication, and individuals often list their names inconsistently across their work (e.g., “Albert Einstein,” “A. Einstein”). Moreover, common names (e.g., “Mary Smith”) may correspond to distinct authors. To overcome these issues, we map instances of authorship to authors using identifiers assigned via probabilistic name matching. For patents, we rely on the “inventor_ids” included with the USPTO data, which are assigned using a machine learning based algorithm. For papers, no probabilistic identifier is included with the data, and therefore we implement our own, unsupervised algorithm, based on a previously described technique [Schulz et al., 2014].

2.3 Knowledge Networks

For the USPTO data, we constructed weighted networks for each year representing the co-occurrence of USPC knowledge classification codes within patents. For APS, we constructed a similar weighted network in each year with the edge weights corresponding to co-occurrence of PACS codes within articles. More formally, let $K^c_y = (V^c_y, E^c_y, w_K)$ represent the a network in year $y$ of subcategory $c$ with weight function $w_K$ acting on the edges. Here, $y \in [1975, 2012]$ and possible values of $c$ are listed in Table 1. Letting $V$ represent all knowledge areas across both datasets, the set $V^c_y \subset V$ represents the knowledge areas cited by all works of subcategory $c$ within year $y$. Note that the patent knowledge areas in $V^c_y$ are not distinct across subcategories or years, such that networks of two different subcategories could contain nodes that represent the same knowledge area.

We define $w_K : E^c_y \rightarrow \mathbb{R}$ as the inverse of the number of co-occurrences between any two knowledge areas across all works in year $y$ and subcategory $c$. This edge weighting represents the pairwise distances among knowledge areas in the network, so that knowledge areas co-occurring more frequently in works are closer than two knowledge areas that are less frequently co-cited in works. With this distance structure, we computed the $k$-dimensional persistent homology for each subcategory network in each year.

2.4 Collaboration Networks

For the USPTO and APS data, we constructed weighted networks for each subcategory representing the co-authorship frequency of authors within the dataset for a particular year with a sliding window. We constructed collaboration networks with both 1 and 3-year sliding windows to align with past work and to match the 1-year sliding window of the knowledge networks. Let $C^c_{i,y} = (A^c_{i,y}, P^c_{i,y}, w_C)$ represent the network in year $y$ with lookback window $i$ of subcategory $c$ with weight function $w_C$ acting on the edges. Here, $y \in [1975, 2012]$, $i \in \{1, 3\}$, and possible values of $c$ are listed in Table 1. Letting $A$ be the set of all authors across both datasets, $A^c_{i,y} \subset A$ represents the authors with works of subcategory $c$ within years $[y-i, y]$. Subsequently, $P^c_{i,y} \subset A^c_{i,y} \times A^c_{i,y}$ represents the relational structure among authors wherein two author nodes are connected by an edge if they were co-authors on a paper in subcategory $c$ in years $[y-i, y]$. Note that the authors $A^c_{i,y}$ are not distinct across subcategories or years.

We define $w_C : P^c_{i,y} \rightarrow \mathbb{R}$ as the inverse of the number of co-authored papers between any two authors for a given $c$, $y$, and $i$. This edge weighting represents the pairwise distances among authors in $C^c_{i,y}$ such that more frequent co-authors are “closer” than less frequent co-authors. With this distance structure, we computed the $k$-dimensional persistent homology for each subcategory network in each year.

3 Interpreting Knowledge Topology

In the conversion of a network to its flag complex, whenever a $k$-clique is formed in the network, we “fill it in” and treat the clique as a higher order topological object: a $(k-1)$-dimensional cell. We may view these higher-order cells as representing abstract knowledge areas composed of $k$ granular knowledge areas. Higher-dimensional homology tracks how these abstract knowledge areas combine, qualifying the meso- and macro-scale structure in the knowledge networks by enumerating the higher-dimensional homology groups
which correspond to “holes.” In the first dimension, \( \beta_0 \) corresponds precisely to the number of connected components of the network. Higher-dimensional holes \( \beta_{i>0} \) imply a relative lack of connectivity across the abstract knowledge areas determined by the \((i+1)\)-dimensional cells, just as \( \beta_0 \) implied a lack of connectivity between clusters of granular knowledge areas. Homology provides a global characterization of structure across the hierarchical representation of knowledge provided by the underlying flag complex of the knowledge network.

Persistent homology tracks this knowledge structure through a filtration on the edge weights of the network, and provides a more granular characterization of this structure across all scales of co-occurrence frequency. The relational structure of the knowledge networks is determined by the frequency of co-occurrence of knowledge areas within works. Using inverse frequency as the filtration parameter, we can view the flag filtration as a discrete assembly of the network wherein the edge connecting the most commonly co-cited knowledge areas is added to the network first, followed by the second most commonly co-cited pair, etc. This construction process continues until the last step in the filtration where edges between knowledge areas with the fewest co-occurrences are added. The interpretation of highly-weighted 1-cells (edges) in the network as pairs of knowledge areas that are frequently combined within works extends to higher dimensions. For example, a 2-cell having high weight on all edges (thus appearing early in the filtration) represents three knowledge areas that are frequently combined within a subfield. Decomposing the flag complex across co-occurrence frequency provides further insight into the meso- and macro-scale structure of these networks apart from their Betti numbers. For example, homology by itself cannot distinguish between a network that retains a large number of connected components up until a small threshold value of co-occurrence frequency in which they all join and a network that grows as a single, dense component across all threshold values. Persistent homology can differentiate these networks, and this difference would be evident in their persistence diagrams.

4 Results

We begin this section by observing the historical dynamics of higher-order structure of both knowledge and collaboration networks across fields. We show that this change in structure is not observable through traditional network-theoretical measures, and that these measures are largely uncorrelated with the homological distribution of the knowledge networks over time. We then move on to relate the topological structure across fields to the nature of the science and technology they produce. We find a striking relationship between higher-order complexity and the abstractness of words used within fields across time. Finally, we observe robust relationships between the higher-order structure of knowledge networks and a number of measures related to innovation within papers.

4.1 Increasing Complexity

We observe substantial shifts in the structure of scientific and technological knowledge over the period of our study. Figure 2 gives an overview of these changes by plotting the average number of topological holes by year for six major fields of science and technology (Chemicals, Computers, Drugs, Electrical, Mechanical, and Physics). Averages are based on number of topological holes observed for the constituent subfields. Raw numbers of holes for each subfield are shown in Figure S1. Corresponding plots for cell counts are shown in the inset axes of Figures 2 and S1. The y-axes of all plots are reported on a \( \log_{10} \) scale. Darker lines in each plot correspond to lower-order structure; higher-order structure is indicated by lighter colored lines. For display purposes, we exclude fields and subfields categorized as “other” from our figures, although they are included in our statistical analyses.

Beginning with Figure 2, we observe several noteworthy patterns. Across fields, there is persistent decline in \( \beta_0 \) over time, followed by a leveling off (Computers, Drugs, Electrical, Mechanical) or modest increase (Chemicals, Physics) in more recent years (beginning in the early 2000s). Because \( \beta_0 \) captures the number of connected components in a network, this pattern suggests that with respect to lower-level structure, the knowledge networks of science and technology are becoming more connected over time, a finding that is consistent with observations from prior research.

Turning to \( \beta_1 \), we also observe fairly consistent patterns across fields. Notably, relative to \( \beta_0 \), there is much less change over time; we see modest increases in \( \beta_1 \) in Chemicals, Computers, Drugs, Electrical, and
Figure 2: Knowledge network topology over time at the field level. The main plots track counts of Betti numbers, while the inset plots track cell counts. All y-axes are reported on a log scale. The “Physics” panel is highlighted to indicate the different data source (APS) and publication type (academic papers) relative to those of the other panels (where data come from the USPTO and the publication type is patents). Note that underlying topological features are measured at the subfield level; to generate these field-level plots, we report the average values observed for the constituent subfields.

Mechanical over the study period, typically peaking sometime roughly between the mid-1980s and mid-1990s, before gradually declining to levels similar to those observed in the 1970s. Physics represents an exception to this pattern; there, we observe a dramatic increase in $\beta_1$ beginning in the late 1970s, which ends in a local peak in the early 1980s, after which there a gradual dip, followed by a similarly gradual increase. Given the increase in $\Delta_2$ (triangles) over time, all fields but Chemistry and Drugs have seen an increase in the number of abstract knowledge areas composed by triplets of low-level concepts. The relatively constant value of $\beta_1$ over time implies that either 1-dimensional holes are being created about as often as they are being closed through the creation of abstract knowledge areas, or these knowledge areas are being generated from pre-existing knowledge structures such that few holes are created or closed.

Relative to $\beta_0$ and $\beta_1$, we observe much more variation, both within and between fields, for higher dimensional holes (i.e., $\beta_2$ and $\beta_3$). Beginning with $\beta_2$, the Chemicals, Drugs, and Mechanical fields follow relatively similar trajectories, with moderately large numbers of 2-dimensional holes (compared to other fields), followed by a gradual increase, and then a leveling off or slight decrease. The pattern of change is more dramatic for the Computers, Electrical, and Physics fields, where we observe relatively low counts of $\beta_2$ in the early years, after which are dramatic increases, followed by a leveling off (but no decline). Finally, with respect to 3-dimensional holes, the patterns are generally similar to those of $\beta_2$, but with the notable exception of Drugs, which has a much more dramatic increase, more akin to the fields of Computers, Electrical, and Physics. The dramatic increase in $\beta_2$ and $\beta_3$ in tandem with an increase in $\Delta_3$ and $\Delta_4$ implies that high-level knowledge areas are being created but are only recently becoming synthesized. This is in contrast to the Mechanical field wherein abstract knowledge continues to be constructed (given the increasing cell counts in high dimensions) but without introducing new gaps as implied by the steady $\beta_2$ and $\beta_3$.

Interestingly, increases in higher order structure often coincide with decreases in lower order structure. This pattern is evident in the various “crossovers” between lines tracking holes of different dimensions. Consider Computers, where the relative ranking of holes by commonality changes several times over the study period.
Here, in the 1970s, the most prevalent holes are 1-dimensional, followed by dimensions 0, 2, and 3. By the late 1990s, the ordering has completely shifted, with the most prevalent holes now being those of dimension 2, and followed by dimensions 1, 3, and 0. This inverse relationship between higher and lower order structure is important because it suggests not only that discovery may be increasingly playing out at higher levels, but also that it is doing less so at lower levels and may therefore be less visible using traditional techniques. Overall, then, these patterns are consistent with our claims on the growing importance of higher-order structure in the knowledge networks of science and technology.

Turning to Figure S1, we observe generally similar patterns at the subfield level. In particular, we see the shift away from lower order structure to higher order structure play out across many different and diverse subfields, as evidenced by the dramatic crossovers in lines tracking different dimensions of holes. There are also, however, several interesting departures from the general patterns. For example, while by the end of the study window, many subfields have noteworthy counts of 3-dimensional holes, there is substantial variation in when those holes appear. Interestingly, the field of Organic Compounds seems to buck the general transition to higher order structure; over the study period, we generally see lower-dimensional holes becoming more prevalent.

Notwithstanding their close mathematical connection, as shown in the inset axes, the patterns of change we observe in cell counts over time are distinctive from those we observe for topological holes. In contrast to what we observe for holes, the relative distributions of cell counts remain fairly stable over time; we see fewer crossovers, and the relative ranks of holes by commonality tends to correspond closely to dimension (with higher dimensional holes being the most common). The overall trajectories of the Computers, Electrical, Mechanical, and Physics fields are fairly similar, being fairly stable in earlier years, followed by a dramatic period of growth, and the subsequent leveling off (Computers, Physics) or decline (Electrical, Mechanical).

Interestingly, shifts in the structure of scientific and technological knowledge from lower- to higher-order structure often coincide with major events in the history of the underlying fields. Consider, for example, the Computers and Electrical fields, which experienced particularly dramatic growth in higher order structure from the early-1980s through the mid-1990s. For both fields, the period was one of dramatic technological change, witnessing the invention of flash memory (1980), the scanning tunneling microscope (1981), World Wide Web (1990), carbon nanotube (1991), and the introduction of the Mosaic web browser (1993). The Drugs field also offers a telling illustration. There, the dramatic increase in higher order structure (particularly 3-dimensional holes) maps closely to major breakthroughs in biotechnology, including marketing of the first recombinant DNA drug (Humulin, 1983) and the invention of the polymerase chain reaction (PCA, 1983), among others.

Figure 2 plots the homology of each knowledge network, aggregated at the NBER field level for the USPTO data, over time. The higher-order structure of these knowledge networks has shown sharp increases over the time period of interest. Also of note is the general downward trend in $\beta_0$, implying that knowledge areas are becoming increasingly connected, coalescing around fewer connected components which may be viewed as large, independent sub-fields within the knowledge area. All fields appear to undergo a tempering or saturation in the growth of their high-dimensional complexity at different points in the time series.

This sharp increase in the higher-order structure of knowledge networks over time is especially interesting when contrasted with the much more tempered growth of higher-order structure in the associated collaboration networks for these fields over the same time period. Figure S2 shows scientists and technologists are increasingly forming higher-order collections of collaborative groups across fields, but the growth in collaboration patterns does not match the growth in the complexity of knowledge produced by these collaborations. At the subcategory level, Figure S3 reinforces this observation, showing many fields have only recently seen emergence in structure in $\beta_2$ and $\beta_3$. Interestingly, the number of connected groups of researchers ($\beta_0$) appears to be stable or increasing slightly over time. This is in contrast to the generally declining number of connected knowledge areas observed in the knowledge networks (Figure 2). These results beg the question as to what extent scientific and technological innovation may be bottlenecked by a lack of complexity in collaborative networks.

To ensure the above historical trends are not a feature of the knowledge network construction itself or whether all two-mode networks of this size show these dynamics, we repeated these historical analyses on a completely different source of knowledge networks constructed via question category tags across a number of Stack Exchange sites. Notably, we observe a slight upward trend in complexity over time, but this growth in complexity is much slower than that of the science and technology networks presented above. See the
4.2 Diverging Topologies

Given the increase in higher-dimensional topological structure over time, we would like to know the extent to which individual knowledge areas show divergence in their topological structure. To do this, we compute the Wasserstein distance (Equation 1) between persistence diagrams in a pairwise fashion between each knowledge subcategory in each year. While individual knowledge areas may converge in their topological similarity across a number of years, the higher-order topological structure between knowledge areas points to divergence over time. Panel A in Figure 3 depicts the average Wasserstein distance across all subcategory pairs in a given year with inset plots showing individual dimensions plotted on their own scale. Clearly, knowledge subcategories differ most in their 1-dimensional persistent homology, which had grown in divergence until the mid-2000’s. In more recent years, topological divergence between knowledge has increased in higher dimensions. These results, combined with the homological trends over time, imply that not only is technological and scientific knowledge getting more topologically complex over time, but this complexity is also diverging in structure across knowledge areas.

Given the increasing and divergent topological complexity of knowledge, we ask whether this increasing complexity is reflected in the author-inventor collaboration structure that produces these knowledge networks. Panel B of Figure 3 plots the average distance between the knowledge and (3-year) collaboration network persistence diagrams within each subcategory and across time. Individual dimensions are again plotted in the inset. Clearly, the difference in topology between the collaboration and knowledge networks has increased rapidly over the entire time series, leveling out only recently. In other words, the collaborative structure of scientists and technologists has severely lagged the knowledge structure produced by these collaborations in topological complexity. Only in the past decade has the higher-order structure of collaboration networks begun to increase (Figure S2). This increase in higher-order collaborative structure may be driven at least in part by the growing complexity of knowledge, as progress on open problems more and more requires attention from larger teams of researchers with expertise spanning multiple domains [Wuchty et al., 2007, Porter and Rafols, 2009, Varga, 2019].
Figure 4: Correlations between knowledge network topology and some popular network-theoretical measures. All correlations are statistically significant at the $p < 0.05$ level with the exception of isolates / nodes ($\beta_1$), modularity ($\Delta_0$), degree assortativity ($\Delta_0$), communities ($\Delta_1$), bridges ($\beta_3$, $\Delta_4$), edges ($\beta_0$), path efficiency ($\beta_1$), and density ($\beta_2$, $\Delta_3$). As expected, network-theoretical measures that approximate global connectivity like path efficiency and degree centralization show higher correlation with higher-dimensional Betti numbers, but this correlation is modest and inverts in lower dimensions. Many of the traditional network-theoretical measures are uncorrelated with higher-dimensional homology. Clearly, the homological information is distinct from the network-theoretic measures and cannot be described by these lower-level network properties.

4.3 Bivariate Network Associations

Figure 4 visualizes correlations between our measures of knowledge network topology (x-dimension) and several more common measures of network structure (y-dimension). The order of the rows (i.e., standard network measures) was determined using a hierarchical clustering algorithm, such that measures that show similar patterns of correlation with topological properties appear adjacent to one another. As may be expected, counts of nodes and edges are among those most strongly associated with knowledge network topology. Most other measures show relatively low correlation. Notably, the correlations with network density are relatively low, which suggests that the emergence of higher order structure is unlikely an artifact of changes in overall network connectivity over time. We also observe that correlations with clustering are relatively low, which is also reassuring given that there are some conceptual similarities between triadic closure and (lower order) measures of network topology. Finally, observe that the correlations between knowledge network topology and measures of community structure. This pattern is noteworthy because community detection is arguably one of the few widely used measures that captures some dimension of higher order structure. Taken together, these results are suggestive that knowledge network topology encodes information that is not captured by widely used measures.

4.4 Linguistic Concreteness

To gain additional insight on the meaning of higher order structure, we conducted an analysis in which we systematically evaluated for differences in word usage by publications as a function of the distribution of Betti numbers for their fields and years of publication. We tokenized words within abstracts of the USPTO dataset, classifying words by their parts of speech. See the Supplemental Materials for more information.
Using these data, we then evaluated for differences in word usage. For each part of speech × token, we computed the Spearman rank correlation between the number of patents using each part of speech × token, by subfield × year observations, separately for the four Betti dimensions. Table 2 reports a subset of the results of this analysis, showing the top 10 lemmas with the largest (positive) and statistically significant (p<0.05) Spearman rank correlation by part of speech and Betti dimension. To minimize noise, we limit our reporting to lemmas that appeared in the abstracts of at least at least 1000 patents across the entire sample. We found similar results (not reported, but available on request from the authors) using more complex models, including those that adjust for field and year effects. We also replicated our analysis using patent titles (rather than abstracts) and found similar patterns to those reported here.

The results show noticeable differences in word usage across dimensions. Across all four parts of speech, we observe a clear pattern according to which lower dimensional holes tend to be associated with more concrete lemmas, while higher dimensional holes tend to be associated with more abstract ones. This pattern is particularly clear for nouns. Under β₀, the most predictive lemmas refer to things that are readily perceptible through sight, sound, and touch (e.g., “crank”, “spool”, “shoe”); strikingly, the list of 10 nouns for β₀ includes 3 of the 6 simple machines (“lever”, “wheel”, “pulley”). Under β₁, by contrast, the most strongly associated nouns refer to things that are less immediately perceptible to the senses (e.g., process, property, method). The most predictive nouns for β₀, β₁, and β₂ encompass a mix of concrete and abstract things. Results for verbs, adjectives, and adverbs follow a similar pattern to those observed with nouns. Lower dimensional holes are associated with more concrete lemmas, often indicating direction or motion (e.g., verbs: “swing”, “pivot”, “disengage”; adjectives: “slidable”, “moveable”, “swinging”; adverbs: “forwardly”, “upwardly”, “rotatably”), while higher dimensional holes are associated with more abstract ones that are typically less amenable to sensory perception (e.g., verbs: “base”, “describe”, “contain”; adjectives: “present”, “active”, “more”; adverbs: “highly”, “significantly”, “specifically”).

In supplemental analyses, we explored differences in the use abstract versus concrete terms across Betti dimensions more systematically by assigning each lemma in our data a concreteness score, using ratings Brysbaert et al. [2014]. We then pulled the lemmas that were significantly (p<0.05) and positively associated with each Betti dimension and computed their average concreteness by dimension and part of speech (Figure S4). Consistent with our observations above, we find that across all four parts of speech, mean concreteness declines with increases in dimension.

We also observe that many of the lemmas most associated with higher-dimensional holes are indicative of engagement with (particularly improvements on) prior knowledge. This pattern is particularly clear for verbs, where the lemmas most strongly associated with β₁ include “base”, “enhance”, “improve”, “add”, “use”, and “modify”. We also see some clear evidence of this pattern with adverbs, where “highly”, “efficiently”, “significantly”, and “optionally” are among the lemmas most strongly associated with β₁.

This increase in abstractness of language with increasing high-dimensional structure aligns with our hypothesized intuition regarding the interpretation high-order structure within knowledge networks (Section 3). High-dimensional holes are created through the adjunction of high-dimensional cells, which themselves are composed of a number of granular knowledge areas represented by nodes, and growth in the creation and combination of high-order cells gives rise to high-dimensional structure as measured by the Betti numbers of the network. The results described in this section imply that as scientists and technologists combine granular knowledge areas into abstract knowledge at the level of cells, the language they use mimics this move to abstraction, as they grapple with the complexities implicit in leveraging multiple distinct knowledge areas within a single work.

### 4.5 Regression

While our results point to dramatic growth in the topological complexity of scientific and technological knowledge, the implications of this growth for future discovery and innovation are less clear. On the one hand, larger numbers of higher dimensional holes may indicate that future advances will hinge on addressing increasingly difficult and perhaps intractable problems. On the other hand, topological complexity may also create opportunities for making new kinds of breakthroughs, allowing investigators to see and do things not possible when working within the confines of a lower dimensional knowledge network.

To evaluate these possibilities, we ran a series of linear regression models that predicted the probability of a publication being in the top 5% of the citation distribution as a function of the topological properties of its
field. Following prior work, our presumption is that high citation counts are likely indicative of breakthroughs; we recognize however that citations are an imperfect proxy, and below we demonstrate consistent results using alternative measures.

For patents, we measure topological properties based on the year of application, which more closely corresponds to the time of invention than grant year; for papers, we match based on the year of publication. The primary predictors of interest—measured at the field × year level—are counts of holes by dimension (i.e., $\beta_0$, $\beta_1$, $\beta_2$, $\beta_3$), which we log transform to account for diminishing effects of large counts. We also included counts of cells by dimension, (i.e., $\Delta_0$, $\Delta_1$, $\Delta_2$, $\Delta_3$; also log transformed), standard measures of network structure from prior work (i.e., density, clustering, and path efficiency), and a measure of publication volume, again all measured at the field × year level. To account for additional confounding factors, our models include fixed effects for each field and year. All tests of statistical significance are based on heteroskedasticity-robust standard errors. Table 3 shows descriptive statistics for the variables in the models.

Coefficient estimates for the regression analysis are shown in Table 4. To facilitate interpretation, Figure 5 plots these estimates for $\beta_0$ through $\beta_3$ based on Table 4, Model 5. We observe a curvilinear (inverted-U shaped) relationship between knowledge network topology and the probability of a hit publication. Increases in 0-dimensional holes ($\beta_0$) are negatively associated with the probability of a hit publication (coef. $= -0.0031; P < 0.001$). Higher dimensional holes ($\beta_1$, $\beta_2$, $\beta_3$) are all positively (and significantly) associated with the probability of a hit, with the magnitude of the coefficient being largest for $\beta_1$ (coef. $= -0.0163; P < 0.001$) and declining thereafter. Overall, this pattern of results offers some support for both views discussed above; increasing topological complexity is associated with breakthroughs, but primarily at moderate dimensionality.

We conducted several analyses to evaluate the predictive power of topological properties relative to common measures in the literature. First, the bottom of Table 3 reports Wald tests that evaluate whether the inclusion of topological measures improves model fit. Across all models, including those with field fixed effects, year fixed effects, and control variables, the null hypothesis is rejected and we conclude that fit improves significantly with the inclusion of the topological measures. Second, we decomposed the adjusted-$R^2$ of Model 5 in Table 3 (our primary model of interest) to evaluate the relative contribution of six groups of predictors—Betti numbers, cell counts, network properties, publication volume, and field and year fixed effects. The results of this analysis are summarized in Table 5. As may be expected, the most informative predictor of a “hit” is the field of publication. However, among the remaining groups of predictors, the Betti numbers (i.e., $\beta_0$, $\beta_1$, $\beta_2$, and $\beta_3$) contribute the most (14.63%) to the adjusted $R^2$; of note, this contribution is roughly 40% more than that made by the basic (lower level) network properties and 43% more than that made by the year fixed effects.

We found that the relationship between knowledge network topology and the probability of a “hit” publication is robust to alternative model specifications. First, we examined whether our results are robust to alternative lags between knowledge network topology and hit publication probability. Table S1 presents models analogous to those of Table 4 but with topological properties measured at time $t - 1$; the pattern of results are similar to those of our main model specifications. Second, for reasons of interpretability and computation, we estimate our statistical models using OLS; however, we also found similar results using nonlinear models (not reported but available upon request). Finally, we repeated all of the statistical analyses discussed above with the exclusion of the APS data (i.e., using patents alone). The results of these supplemental analyses are shown alongside our main analyses (i.e., those using both samples) in the supplemental appendix. While there are some minor differences in various specifications, the overall pattern of results is remarkably similar.

We also conducted several additional analyses (reported in Table 6) to help better understand the implications of topological complexity for discovery and innovation. Models 1 and 2 of Table 6 evaluate the relationship between knowledge network topology and the search depth of publications. If topological complexity creates opportunities for new kinds of breakthroughs, then increases in such complexity may prompt investigators to comb more deeply through prior work for potential solutions. We consider two proxies for search depth, (1) the ratio of self-citations to total citation and (2) the variation in the age of prior work cited and citation age variation. Our presumption is that higher values of both the former and latter will reflect lesser and greater search depth, respectively. Figure 6 plots coefficient estimates for the Betti numbers ($\beta_0$, $\beta_1$, $\beta_2$, and $\beta_3$) from these models. The results are consistent with our expectations; at higher dimensions, increases in holes are associated with fewer self citations, while the corresponding pattern for citation age variation is inverted-U shaped.
Models 4 and 5 evaluate the relationship between knowledge network topology and the novelty of publications. Paralleling our thinking on search depth, if topological complexity creates opportunities for new kinds of breakthroughs, then increases in such complexity may prompt investigators to try out ideas that are more distinctive vis-a-vis what has been done before. While novelty may manifest in any number of ways, we consider two proxies, (1) new subclass combinations and (2) the Jensen-Shannon divergence (i.e., surprisal) of publications based on the distribution of word frequencies in their abstracts. Once again, we observe results that are consistent with the idea that up to a point, increasing topological complexity may be generative of discovery and innovation (see Figure 6 for coefficient plots).

Finally, Models 3 and 6 of Table 6 evaluate the relationship between knowledge network topology and publication complexity. If topological complexity creates opportunities for new kinds of breakthroughs, then increases in such complexity may prompt investigators to try out ideas that are themselves more complex. As with search depth and novelty, we consider two proxies for complexity, (1) delayed recognition (i.e., publications that are slower to gain citations) and (2) lexical diversity (i.e., more unique words per total word). Our rationale for the former proxy was based on the idea that the significance of more complex publications should be more difficult to recognize, and thereby take longer for future work to use; for the latter proxy, our motivation was based on the idea that describing more complex ideas is likely to require more diverse vocabularies. Results (see Figure 6 for coefficient plots) from these analyses are consistent with our expectations. Increases in higher dimensional holes are positively associated with delayed recognition; the relationship between holes and lexical diversity is U-shaped, with increases in the highest dimensional holes being associated with increases in diversity.

5 Discussion

For decades, scientific and technological knowledge has developed at a historically unprecedented pace. Yet observers have also questioned whether such progress is sustainable. Recently, network science has emerged as a powerful framework for measuring the structure and dynamics of knowledge, and findings from this work lend some credence to concerns of slowing progress. However, current approaches are limited because they overlook the higher-order structure of knowledge, instead focusing on lower-level, dyadic interactions among components. Thus, observations of slowing progress in science and technology may in part be due to the shifting locus of discovery and invention to higher dimensions, which require new lenses to observe.

We drew on methods from algebraic topology to map the dynamic, higher-order structure of knowledge in science and technology. Our analysis led to several noteworthy findings. First, we documented the historical emergence of higher-order structure across diverse fields of science and technology. Interestingly, the growth of higher-order structure often coincides with the decline of lower-order structure. We further demonstrated that the emergence of higher-order structure in knowledge networks is happening alongside the emergence of higher-order structure in scientific and technological collaboration networks; though growth in the former is outpacing growth in the latter, and the topologies of the two categories of networks (knowledge and collaboration) are diverging over time. The knowledge-structural topology of fields also tends to be diverging, implying the way in which knowledge is brought together across fields is becoming increasingly heterogeneous.

Second, we observe that topological structure is related to the nature of the science and technology produced. As the preponderance of higher dimensional holes increases, publications tend to use language that is more abstract, developmental, and also—at least up to a point—more diverse and novel. These observations are consistent with the idea that moderate levels of higher-order structure may be generative of discovery and invention. Our findings of a curvilinear (inverted-U shaped) relationship between further underscore this interpretation.

Finally, we demonstrated that the topological structure of scientific and technological knowledge encodes information that is not captured by existing measures and models. Associations between our measures of higher-order structure and common, lower-order measures of network characteristics are typically low. Moreover, the variation in higher-order structure we observe cannot be described by simple small-world or preferential-attachment models. This finding suggests that the patterns we observe are unlikely to be artifacts of the data or underlying network structure. We further demonstrated that the distribution of topological holes in the knowledge network of a field is more predictive of hit publications than a host of other factors, including lower-order network measures. Taken together, these results provide compelling evidence that our
measures of higher order structure capture variation that is not captured using current approaches.

Our findings should be understood within the context of several limitations. First, while our assessments of knowledge networks in technology were based on all patents granted by the USPTO, our analysis of science was limited to journals published by the APS. Thus, more work needs to be done to evaluate whether and to what degree our findings using the APS data generalize to larger databases that cover a broader array of academic disciplines. Second, although our findings suggest that algebraic topology offers an exciting new lens for the study of knowledge networks, computational constraints currently limit their application to very large databases. Finally, our regression analyses are based on observational data, and therefore our findings on the relationship between higher-order structure and various outcomes should not be interpreted as indicating causal relationships.

Notwithstanding these limitations, our study has several implications both for future research and science policy. First, our findings suggest the need to rethink and deepen theories of invention in science and technology. Classical theories describe invention as a process of recombination, in which existing components of knowledge are brought together in novel configurations. These theories are typically not attentive to the dimensionality of the components brought together. Yet our results suggest that dimensionality of knowledge may be important for shaping both the opportunities for and challenges of recombination. Bringing together similar knowledge components but at different levels of dimensionality may, for example, require distinctive creative processes, resulting in qualitatively distinctive inventions. Second, our results suggest the opportunity for more exploration of models of higher order structure in other networks of interest in Science of Science. While our primary focus was on knowledge networks, several of our analyses pointed to important changes in the topological structure of collaboration networks, with higher order structure becoming more prevalent (though not to the same degree as observed for knowledge networks). Theories of invention suggest that social network position is an important determinant of individual creativity, with positions that span holes in social structures being particularly valuable. While this view is intuitively attractive, empirical work has produced a myriad of conflicting findings. Yet prior work has not considered the possibility that the benefits of spanning a structural hole are contingent on its dimensionality. Such a possibility may offer one approach for reconciling these conflicting results.

References

Daron Acemoglu, Ufuk Akcigit, and William R Kerr. Innovation network. *Proceedings of the National Academy of Sciences*, 113(41):11483–11488, 2016.

Ajay Agrawal, Avi Goldfarb, and Florenta Teodoridis. Understanding the changing structure of scientific inquiry. *American Economic Journal: Applied Economics*, 8(1):100–128, 2016.

Mehmet E Aktas, Esra Akbas, and Ahmed El Fatmaoui. Persistence homology of networks: methods and applications. *Applied Network Science*, 4(1):61, 2019.

Samuel Arbesman. Quantifying the ease of scientific discovery. *Scientometrics*, 86(2):245–250, 2011.

Albert-László Barabási and Réka Albert. Emergence of scaling in random networks. *Science*, 286(5439):509–512, 1999.

Ulrich Bauer. Ripser: efficient computation of vietoris-rips persistence barcode, August 2019. Preprint.

Nicholas Bloom, Charles I Jones, John Van Reenen, and Michael Webb. Are ideas getting harder to find? *American Economic Review*, 110(4):1104–44, 2020.

Marc Brysbaert, Amy Beth Warriner, and Victor Kuperman. Concreteness ratings for 40 thousand generally known english word lemmas. *Behavior research methods*, 46(3):904–911, 2014.

Gunnar Carlsson. Topology and data. *Bulletin of the American Mathematical Society*, 46(2):255–308, 2009.

Nicolas H Christianson, Ann Sizemore Blevins, and Danielle S Bassett. Architecture and evolution of semantic networks in mathematics texts. *Proceedings of the Royal Society A*, 476(2239):20190741, 2020.
Johan SG Chu and James Evans. Too many papers? slowed canonical progress in large fields of science. 2018.

David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Stability of persistence diagrams. *Discrete & computational geometry*, 37(1):103–120, 2007.

Tyler Cowen. *The great stagnation: How America ate all the low-hanging fruit of modern history, got sick, and will (eventually) feel better: A Penguin eSpecial from Dutton*. Penguin, 2011.

Tyler Cowen and Ben Southwood. Is the rate of scientific progress slowing down? Technical report, 2019.

Jordan D Dworkin, Russell T Shinohara, and Danielle S Bassett. The emergent integrated network structure of scientific research. *PloS one*, 14(4):e0216146, 2019.

Paul Erdős and Alfréd Rényi. On random graphs i. *Publ. Math. Debrecen*, 6(290-297):18, 1959.

Lee Fleming. Recombinant uncertainty in technological search. *Management science*, 47(1):117–132, 2001.

Jacob G Foster, Andrey Rzhetsky, and James A Evans. Tradition and innovation in scientists’ research strategies. *American Sociological Review*, 80(5):875–908, 2015.

Robert Christ. Barcodes: the persistent topology of data. *Bulletin of the American Mathematical Society*, 45(1):61–75, 2008.

Robert J Gordon. *The rise and fall of American growth: The US standard of living since the civil war*, volume 70. Princeton University Press, 2017.

A. Hatcher, Cambridge University Press, and Cornell University. Dept. of Mathematics. *Algebraic Topology*. Cambridge University Press, 2002. ISBN 9780521795401.

Benjamin F Jones. The burden of knowledge and the “death of the renaissance man”: Is innovation getting harder? *The Review of Economic Studies*, 76(1):283–317, 2009.

Benjamin F Jones. Age and great invention. *The Review of Economics and Statistics*, 92(1):1–14, 2010.

Erin Leahey, Christine M Beckman, and Taryn L Stanko. Prominent but less productive: The impact of interdisciplinarity on scientists’ research. *Administrative Science Quarterly*, 62(1):105–139, 2017.

Daniel Lütgehetmann, Dejan Govc, Jason P Smith, and Ran Levi. Computing persistent homology of directed flag complexes. *Algorithms*, 13(1):19, 2020.

Staša Milojević. Quantifying the cognitive extent of science. *Journal of Informetrics*, 9(4):962–973, 2015.

Satyam Mukherjee, Brian Uzzi, Ben Jones, and Michael Stringer. A new method for identifying recombinations of existing knowledge associated with high-impact innovation. *Journal of Product Innovation Management*, 33(2):224–236, 2016.

Nina Otter, Mason A Porter, Ulrike Tillmann, Peter Grindrod, and Heather A Harrington. A roadmap for the computation of persistent homology. *EPJ Data Science*, 6(1):17, 2017.

Raj K Pan, Alexander M Petersen, Fabio Pammolli, and Santo Fortunato. The memory of science: Inflation, myopia, and the knowledge network. *Journal of Informetrics*, 12(3):656–678, 2018.

Alan Porter and Ismael Rafols. Is science becoming more interdisciplinary? measuring and mapping six research fields over time. *Scientometrics*, 81(3):719–745, 2009.

Andrey Rzhetsky, Jacob G Foster, Ian T Foster, and James A Evans. Choosing experiments to accelerate collective discovery. *Proceedings of the National Academy of Sciences*, 112(47):14569–14574, 2015.

Christian Schulz, Amin Mazloumian, Alexander M Petersen, Orion Penner, and Dirk Helbing. Exploiting citation networks for large-scale author name disambiguation. *EPJ Data Science*, 3(1):11, 2014.
J.A. Schumpeter. *The Theory of Economic Development: An Inquiry Into Profits, Capital, Credit, Interest, and the Business Cycle*. Economics Third World studies. Transaction Books, 1983. ISBN 9780878556984.

Feng Shi, Jacob G Foster, and James A Evans. Weaving the fabric of science: Dynamic network models of science’s unfolding structure. *Social Networks*, 43:73–85, 2015.

Brian Uzzi, Satyam Mukherjee, Michael Stringer, and Ben Jones. Atypical combinations and scientific impact. *Science*, 342(6157):468–472, 2013.

Attila Varga. Shorter distances between papers over time are due to more cross-field references and increased citation rate to higher-impact papers. *Proceedings of the National Academy of Sciences*, 116(44):22094–22099, 2019.

Duncan J Watts and Steven H Strogatz. Collective dynamics of ‘small-world’networks. *Nature*, 393(6684):440–442, 1998.

Lingfei Wu, Dashun Wang, and James A Evans. Large teams develop and small teams disrupt science and technology. *Nature*, 566(7744):378–382, 2019.

Stefan Wuchty, Benjamin F Jones, and Brian Uzzi. The increasing dominance of teams in production of knowledge. *Science*, 316(5827):1036–1039, 2007.
Figure 5: Plots of coefficients from regression predicting “hit” publications

Betti numbers. This figure visualizes coefficient estimates for Betti numbers from Table 4 (Model 5). Error bars represent 95 percent confidence intervals. Error bars that span 0 indicate that the corresponding coefficient is not significantly different from 0; coefficients with overlapping error bars may however be significantly different from each other.
Figure 6: Coefficient estimates for Betti numbers from Table 6. Model numbers are given above each plot. Error bars represent 95 percent confidence intervals. Error bars that span 0 indicate that the corresponding coefficient is not significantly different from 0; coefficients with overlapping error bars may however be significantly different from each other.
| Subcategory Name        | Field          | Total Articles | Max Articles | Max Article Year | Min Articles | Min Article Year | Mean Articles/Year |
|-------------------------|----------------|----------------|--------------|------------------|--------------|------------------|-------------------|
| Agriculture             | Chemicals      | 18934          | 725          | 1989             | 272          | 2008             | 541               |
| Coating                 | Chemicals      | 51431          | 2297         | 2000             | 778          | 1979             | 1469              |
| Gas                     | Chemicals      | 16401          | 898          | 2010             | 290          | 1979             | 469               |
| Organic compounds       | Chemicals      | 104231         | 5465         | 1976             | 2135         | 2005             | 2978              |
| Resins                  | Chemicals      | 110505         | 4312         | 2001             | 1977         | 1979             | 3157              |
| Communications          | Computers      | 277240         | 24160        | 2010             | 1663         | 1979             | 791               |
| Hardware and software   | Computers      | 368020         | 35572        | 2014             | 1014         | 1979             | 9200              |
| Computer peripherals    | Computers      | 96753          | 8713         | 2010             | 285          | 1979             | 2764              |
| Information storage     | Computers      | 128085         | 11313        | 2010             | 631          | 1979             | 3660              |
| Business methods        | Computers      | 42137          | 7803         | 2010             | 37           | 1979             | 1204              |
| Drugs                   | Drugs          | 204220         | 11275        | 2010             | 1781         | 1979             | 5835              |
| Surgery                 | Drugs          | 120046         | 7573         | 2010             | 784          | 1979             | 3430              |
| Genetics                | Drugs          | 27613          | 1579         | 2010             | 227          | 1978             | 789               |
| Electrical devices      | Electrical     | 129274         | 6861         | 2010             | 1490         | 1979             | 3694              |
| Electrical lighting     | Electrical     | 68555          | 4363         | 2010             | 733          | 1979             | 1959              |
| Measuring and testing   | Electrical     | 114823         | 5848         | 2010             | 1488         | 1979             | 3281              |
| Nuclear and x-rays      | Electrical     | 58667          | 3134         | 2010             | 718          | 1979             | 1676              |
| Power systems           | Electrical     | 146737         | 9616         | 2010             | 1709         | 1979             | 4192              |
| Semiconductor devices   | Electrical     | 164486         | 14813        | 2010             | 495          | 1979             | 4700              |
| Material processing     | Mechanical     | 156396         | 5769         | 2001             | 3044         | 1979             | 4468              |
| Metal working           | Mechanical     | 93232          | 3509         | 2001             | 1782         | 1979             | 2664              |
| Motors and engines      | Mechanical     | 125247         | 5250         | 2002             | 1924         | 1979             | 3578              |
| Optics                  | Mechanical     | 60978          | 3884         | 2006             | 588          | 1982             | 1742              |
| Transportation          | Mechanical     | 105559         | 4886         | 2010             | 1567         | 1979             | 3016              |
| APS                     | Physics        | 739004         | 38054        | 2010             | 9362         | 1980             | 23839             |

Notes: High-level statistics of USPTO and APS computed across the years of interest 1976-2010. Subcategory Name corresponds to the NBER subcategory classification name for the USPTO data.
| Lemma     | \( \beta_0 \) | \( \beta_1 \) | \( \beta_2 \) | \( \beta_3 \) |
|-----------|----------------|----------------|----------------|----------------|
| crank     | 0.70           | 0.71           | process        | 0.75           |
| lever     | 0.67           | condition      | 0.71           | property       | 0.72           |
| rearwardly| 0.64           | ring           | 0.71           | step           | 0.71           |
| pulley    | 0.64           | carrier        | 0.71           | method         | 0.71           |
| spool     | 0.64           | case           | 0.70           | degradation    | 0.71           |
| shoe      | 0.63           | use            | 0.70           | substrate      | 0.70           |
| clutch    | 0.63           | pressure       | 0.69           | functionality  | 0.69           |
| sprocket  | 0.62           | reduction      | 0.69           | amount         | 0.69           |
| engagement| 0.62           | degree         | 0.68           | medium         | 0.68           |
| wheel     | 0.62           | strength       | 0.68           | invention      | 0.68           |

| Lemma     | \( \beta_0 \) | \( \beta_1 \) | \( \beta_2 \) | \( \beta_3 \) |
|-----------|----------------|----------------|----------------|----------------|
| swing     | 0.62           | carry          | 0.74           | contain        | 0.71           |
| pivot     | 0.62           | say            | 0.72           | describe       | 0.71           |
| actuate   | 0.62           | comprise       | 0.72           | improve        | 0.70           |
| journaled | 0.60           | have           | 0.71           | base           | 0.69           |
| disengage | 0.60           | form           | 0.70           | enhance        | 0.69           |
| coact     | 0.60           | characterize   | 0.70           | use            | 0.68           |
| journaled | 0.60           | bring          | 0.70           | add            | 0.67           |
| hinge     | 0.59           | contact        | 0.69           | result         | 0.67           |
| brake     | 0.59           | separate       | 0.69           | exhibit        | 0.67           |
| grip      | 0.59           | consist        | 0.69           | obtain         | 0.66           |

| Lemma     | \( \beta_0 \) | \( \beta_1 \) | \( \beta_2 \) | \( \beta_3 \) |
|-----------|----------------|----------------|----------------|----------------|
| upstanding| 0.62           | low            | 0.72           | present        | 0.70           |
| slidable  | 0.62           | improved       | 0.71           | less           | 0.70           |
| pivotal   | 0.61           | intermediate   | 0.71           | active         | 0.70           |
| movable   | 0.61           | free           | 0.70           | good           | 0.69           |
| pivotable | 0.60           | such           | 0.70           | mixed          | 0.68           |
| engageable| 0.60           | further        | 0.70           | more           | 0.68           |
| shiftable | 0.60           | same           | 0.69           | excellent      | 0.68           |
| eccentric | 0.60           | suitable       | 0.68           | least          | 0.68           |
| swinging  | 0.60           | other          | 0.68           | non            | 0.68           |
| elongated | 0.59           | double         | 0.68           | stable         | 0.67           |

| Lemma     | \( \beta_0 \) | \( \beta_1 \) | \( \beta_2 \) | \( \beta_3 \) |
|-----------|----------------|----------------|----------------|----------------|
| pivotally | 0.66           | together       | 0.72           | e.g.           | 0.71           |
| forwardly | 0.65           | thereof        | 0.72           | highly         | 0.70           |
| resiliently| 0.64          | continuously   | 0.70           | wherein        | 0.69           |
| adjustably| 0.63           | essentially    | 0.70           | where          | 0.68           |
| upwardly  | 0.62           | whereby        | 0.69           | least          | 0.68           |
| transversely| 0.61         | substantially | 0.68           | optionally     | 0.66           |
| rotatably | 0.61           | relatively     | 0.68           | significantly  | 0.66           |
| lengthwise| 0.60           | directly       | 0.68           | advantageously | 0.64           |
| drivingly | 0.60           | first          | 0.68           | efficiently    | 0.63           |
| rigidly   | 0.60           | where          | 0.68           | about          | 0.63           |

Notes: Parts of speech within USPTO abstracts with highest Spearman correlation with Betti numbers. Note above results are comparable to using OLS and controlling for field.
Table 3: Summary statistics for variables used in regression analyses

| Variable                  | N       | N_unique | Mean  | SD    | Min   | Max    | Level of measurement |
|---------------------------|---------|----------|-------|-------|-------|--------|----------------------|
| **Topological**           |         |          |       |       |       |        |                      |
| $\beta_0$ (log)           | 4283637 | 198      | 3.30  | 1.31  | 0.00  | 5.95   | Field × year          |
| $\beta_1$ (log)           | 4283637 | 755      | 6.17  | 1.14  | 0.00  | 7.91   | Field × year          |
| $\beta_2$ (log)           | 4283637 | 472      | 5.04  | 2.07  | 0.00  | 8.22   | Field × year          |
| $\beta_3$ (log)           | 4278984 | 216      | 3.13  | 2.50  | 0.00  | 7.87   | Field × year          |
| $\Delta_0$ (log)          | 4283637 | 1248     | 8.39  | 1.06  | 0.00  | 9.82   | Field × year          |
| $\Delta_1$ (log)          | 4283637 | 1347     | 10.38 | 1.45  | 0.00  | 12.45  | Field × year          |
| $\Delta_2$ (log)          | 4283637 | 1361     | 11.66 | 2.00  | 0.00  | 15.94  | Field × year          |
| $\Delta_3$ (log)          | 4283637 | 1357     | 12.72 | 2.61  | 0.00  | 19.75  | Field × year          |
| $\Delta_4$ (log)          | 4278984 | 1357     | 13.70 | 3.24  | 0.00  | 23.17  | Field × year          |
| **Outcomes**              |         |          |       |       |       |        |                      |
| Hit publication           | 4283676 | 2        | 0.05  | 0.22  | 0.00  | 1.00   | Publication           |
| Citation age variation    | 3886365 | 611288   | 0.47  | 0.31  | -143.92 | 82.31  | Publication           |
| Self-citation ratio       | 3892496 | 6156     | 0.08  | 0.18  | 0.00  | 1.00   | Publication           |
| Delayed recognition       | 3896371 | 652      | 1.14  | 10.77 | -1007.00 | 2339.00 | Publication           |
| New subclass combinations | 3860383 | 812      | 3.49  | 22.73 | 0.00  | 15867.00 | Publication           |
| Abstract surprisal        | 3847898 | 3786985  | 0.30  | 0.06  | 0.10  | 0.97   | Publication           |
| Abstract lexical diversity| 4116571 | 22422    | 0.54  | 0.13  | 0.06  | 1.00   | Publication           |
| **Controls**              |         |          |       |       |       |        |                      |
| Publications (log)        | 4283637 | 1188     | 8.29  | 1.32  | 0.00  | 10.09  | Field × year          |
| Knowledge network density | 4251206 | 1364     | 0.00  | 0.01  | 0.00  | 1.00   | Field × year          |
| Knowledge network clustering | 4251206 | 1360   | 0.30  | 0.10  | 0.15  | 1.00   | Field × year          |
| Knowledge network path efficiency | 4283637 | 1365 | 0.23  | 0.08  | 0.00  | 1.00   | Field × year          |
| **Fixed effects**         |         |          |       |       |       |        |                      |
| Year                      | 4283637 | 42       | –     | –     | –     | –      | Year                 |
| Field                     | 4283676 | 38       | –     | –     | –     | –      | Field               |
Table 4: Regressions predicting “hit” publications

|                | Sample: USPTO + APS | Sample: USPTO |
|----------------|---------------------|---------------|
|                | (1)                | (2)           |
| $\beta_0$ (log)  | -0.0207***         | -0.0013**     |
|                | (0.0004)           | (0.0004)      |
| $\beta_1$ (log)  | 0.0072***          | 0.0132***     |
|                | (0.0003)           | (0.0005)      |
| $\beta_2$ (log)  | 0.0060***          | 0.0059***     |
|                | (0.0001)           | (0.0002)      |
| $\beta_3$ (log)  | 0.0106***          | 0.0019***     |
|                | (0.0001)           | (0.0002)      |
| $\Delta_0$ (log)| 0.0378***          | -0.0282***    |
|                | (0.0019)           | (0.0040)      |
| $\Delta_1$ (log)| 0.0118**           | 0.0518***     |
|                | (0.0039)           | (0.0061)      |
| $\Delta_2$ (log)| -0.1695***         | -0.0747***    |
|                | (0.0051)           | (0.0062)      |
| $\Delta_3$ (log)| 0.1365***          | 0.0396***     |
|                | (0.0037)           | (0.0040)      |
| $\Delta_4$ (log)| -0.0380***         | -0.0070***    |
|                | (0.0011)           | (0.0012)      |

|                | (3)                | (4)           |
|                | 0.0331***          | 0.0053***     |
|                | (0.0005)           | (0.0005)      |
|                | 0.0163***          | 0.0137***     |
|                | (0.0005)           | (0.0005)      |
|                | 0.0074***          | 0.0059***     |
|                | (0.0002)           | (0.0002)      |
|                | 0.0015***          | 0.0011***     |
|                | (0.0002)           | (0.0002)      |
|                | -0.0427***         | -0.1045***    |
|                | (0.0044)           | (0.0043)      |
|                | 0.0971***          | -0.0022       |
|                | (0.0065)           | (0.0057)      |
|                | -0.1088***         | -0.2262***    |
|                | (0.0066)           | (0.0077)      |
|                | 0.0602***          | 0.2092***     |
|                | (0.0045)           | (0.0057)      |
|                | -0.0191***         | -0.0651***    |
|                | (0.0014)           | (0.0018)      |
|                | 0.0016***          | 0.0394***     |
|                | (0.0012)           | (0.0018)      |

|                | (5)                | (6)           |
|                | 0.0306***          | 0.0053***     |
|                | (0.0004)           | (0.0005)      |
|                | 0.0033***          | 0.0136***     |
|                | (0.0004)           | (0.0005)      |
|                | 0.0078***          | 0.0066***     |
|                | (0.0001)           | (0.0002)      |
|                | 0.0089***          | 0.0011***     |
|                | (0.0001)           | (0.0002)      |
|                | -0.0001            | 0.0001**      |
|                |                   | (0.0001)      |

|                | (7)                | (8)           |
|                | 0.0064***          | 0.0002       |
|                | (0.0002)           | (0.0002)      |
|                | 0.0015***          | 0.0015***     |
|                | (0.0002)           | (0.0002)      |
|                | -0.0969***         | 0.0045**      |
|                | (0.0004)           | (0.0045)      |
|                | 0.1644***          | 0.0072       |
|                | (0.0008)           | (0.0070)      |
|                | -0.2018***         | 0.0081       |
|                | (0.0017)           | (0.0082)      |
|                | 0.1353***          | 0.0058       |
|                | (0.0045)           | (0.0057)      |
|                | -0.0394***         | 0.0018      |
|                | (0.0002)           | (0.0018)      |

|                | (9)                | (10)          |
| Year fixed effects | No  Yes  Yes  Yes  Yes  No  Yes  Yes  Yes  Yes |
| Field fixed effects| No  Yes  Yes  Yes  Yes  No  Yes  Yes  Yes  Yes |
| Controls         | Yes  No  Yes  Yes  Yes  Yes  No  Yes  Yes  Yes |
| N                | 4246553 4246553 4246553 4246553 4246553 3855730 3855730 3855730 3855730 3855730 |
| Adjusted R2      | 0.02 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 0.04 |

Wald tests for topology predictors

|                | (1)                | (2)           |
|                | 4308.74 476.44 878.95 | 435.54        |
| d.f.            | 9.00 9.00 9.00      | 9.00          |
| p-value         | 0.08 0.00 0.00      | 0.08          |

Notes: Estimates are from ordinary-least-squares regressions (linear probability models). This table evaluates the association between knowledge network topology (measured at the level of the field × year) and the probability of a “hit” publication (patent or paper). Hit publications are defined (using a 0/1 indicator variable) as those that are cited more than 95 percent of all other publications across fields and years, as of 5 years after publication. When indicated, included control variables are measures of the number of publications (logged) and knowledge network density for each field × year observation. For more details on variables, see Table 3. Wald tests reported below each model evaluate whether the included topological predictors significantly improve model fit. Robust standard errors are shown in parentheses; p-values correspond to two-tailed tests.

+p<0.1; *p<0.05; **p<0.01; ***p<0.001
Table 5: Decomposition of adjusted $R^2$ from regression models predicting “hit” publications

(a) Sample: USPTO + APS

| Variable set                                                                 | Contribution to adjusted $R^2$ | Raw | Percent | Rank |
|------------------------------------------------------------------------------|--------------------------------|-----|---------|------|
| $\beta_0$ (log), $\beta_1$ (log), $\beta_2$ (log), $\beta_3$ (log)          | 0.0058                         |     | 14.63   | 2    |
| $\Delta_0$ (log), $\Delta_1$ (log), $\Delta_2$ (log), $\Delta_3$ (log), $\Delta_4$ (log) | 0.0050                         |     | 12.69   | 3    |
| Knowledge network density, Knowledge network clustering, Knowledge network path efficiency | 0.0039                         |     | 9.78    | 4    |
| Publications (log)                                                           | 0.0008                         |     | 1.95    | 6    |
| Year fixed effects                                                           | 0.0037                         |     | 9.42    | 5    |
| Field fixed effects                                                          | 0.0205                         |     | 51.54   | 1    |
| N                                                                            | 4246553                        |     |         |      |
| Overall adjusted $R^2$                                                      | 0.0397                         |     |         |      |

(b) Sample: USPTO

| Variable set                                                                 | Contribution to adjusted $R^2$ | Raw | Percent | Rank |
|------------------------------------------------------------------------------|--------------------------------|-----|---------|------|
| $\beta_0$ (log), $\beta_1$ (log), $\beta_2$ (log), $\beta_3$ (log)          | 0.0051                         |     | 13.53   | 2    |
| $\Delta_0$ (log), $\Delta_1$ (log), $\Delta_2$ (log), $\Delta_3$ (log), $\Delta_4$ (log) | 0.0032                         |     | 8.48    | 4    |
| Knowledge network density, Knowledge network clustering, Knowledge network path efficiency | 0.0028                         |     | 7.48    | 5    |
| Publications (log)                                                           | 0.0003                         |     | 0.85    | 6    |
| Year fixed effects                                                           | 0.0048                         |     | 12.81   | 3    |
| Field fixed effects                                                          | 0.0213                         |     | 56.84   | 1    |
| N                                                                            | 3855730                        |     |         |      |
| Overall adjusted $R^2$                                                      | 0.0376                         |     |         |      |

Notes: See Models 5 and 10 of Table 4 for the full regressions underpinning the decompositions in panels (a) and (b) above, respectively.
Table 6: Regressions predicting search depth, novelty, and complexity of publications

|                      | Sample: USPTO + APS | Sample: USPTO |
|----------------------|---------------------|---------------|
|                      | (1)                 | (2)           |
|                      | (3)                 | (4)           |
|                      | (5)                 | (6)           |
| **Self-citation ratio** (Proxy for search depth) | **Citation age variation** (Proxy for search depth) | **Delayed recognition** (Proxy for novelty) | **New subclass combinations** (Proxy for novelty) | **Abstract surprisal** (Proxy for novelty) | **Abstract lexical diversity** (Proxy for complexity) |
| \( \beta_0 \) (log) | 0.0047*** (0.0004)  | -0.0095*** (0.0005) | -0.4582*** (0.0244) | 0.0026 (0.0690) | 0.0016*** (0.0001) | -0.0010*** (0.0003) |
| \( \beta_1 \) (log) | 0.0029*** (0.0008)  | 0.0319*** (0.0009) | 0.1210*** (0.0285) | 1.5614*** (0.0027) | 0.0087*** (0.0002) | -0.0039*** (0.0004) |
| \( \beta_2 \) (log) | -0.0017*** (0.0003) | 0.0070*** (0.0004) | 0.0650*** (0.0099) | 0.2964*** (0.0030) | 0.0026*** (0.0001) | -0.0018*** (0.0001) |
| \( \beta_3 \) (log) | -0.0009*** (0.0002) | -0.0043*** (0.0003) | 0.1389*** (0.0084) | -0.1834*** (0.0209) | -0.0004*** (0.0001) | 0.0011*** (0.0001) |
| \( \Delta_0 \) (log) | 0.0144* (0.0057)   | 0.0001 (0.0060) | 1.6051*** (0.2050) | -3.0818+ (1.6305) | -0.159*** (0.0015) | 0.1028*** (0.0031) |
| \( \Delta_1 \) (log) | -0.0126 (0.0094)   | -0.1465*** (0.0092) | -4.5364*** (0.2940) | -9.1558+ (4.7986) | -0.0120*** (0.0001) | -0.1031*** (0.0052) |
| \( \Delta_2 \) (log) | 0.0360*** (0.0098) | 0.0696*** (0.0096) | 2.0355*** (0.2653) | 13.9286* (5.9577) | 0.0119*** (0.0027) | 0.0288*** (0.0058) |
| \( \Delta_3 \) (log) | -0.0284*** (0.0063) | -0.0064 (0.0065) | -0.4039* (0.1620) | -7.4918* (3.6221) | -0.0036+ (0.0019) | 0.0011 (0.0040) |
| \( \Delta_4 \) (log) | 0.0103*** (0.0019) | 0.0000 (0.0020) | -0.1336* (0.0503) | 1.8002* (0.9110) | 0.0016** (0.0006) | -0.0022+ (0.0012) |

Year fixed effects: Yes | Yes | Yes | Yes | Yes | Yes | Yes
Field fixed effects: Yes | Yes | Yes | Yes | Yes | Yes | Yes
Controls: Yes | Yes | Yes | Yes | Yes | Yes | Yes
N: 2956056 | 3852420 | 3859287 | 3855730 | 3843247 | 3843249 |
Adjusted R2: 0.05 | 0.21 | 0.06 | 0.01 | 0.19 | 0.16

Notes: Estimates are from ordinary-least-squares regressions (linear probability models). This table evaluates the association between knowledge network topology (measured at the level of the field x year) and proxies for the search depth, novelty, and complexity of publications (patents and papers). Included control variables are measures of the number of publications (logged) and knowledge network density for each field x year observation. Model 1 is conditional on the possibility of self-citation (i.e., at least one member of the author team must have published previously). For more details on variables, see Table 3. Robust standard errors are shown in parentheses; p-values correspond to two-tailed tests.

+ p < 0.1; * p < 0.05; ** p < 0.01; *** p < 0.001
6 Supplementary Materials

6.1 Methods

6.1.1 Persistence Computation

For all networks, we computed persistent homology using the Flagser package [Lütgehetmann et al., 2020]. Although originally designed to compute persistent homology of directed flag complexes, the package provides good performance in the computation of persistent homology on undirected flag complexes as well. Flagser is built on top of Ripser [Bauer, 2019], a high-performance C++ package for computing Vietoris-Rips persistence, and provides high-level improvements to memory management, filtration customization, approximations, and input/output. Computing persistent homology is a high-complexity operation in terms of both computation and memory. The computational complexity of persistent homology is at worst cubic in the number of cells in a particular dimension and is believed to be on the order of matrix multiplication, as the persistence calculation is intrinsically a matrix decomposition of boundary matrices [Otter et al., 2017]. Unfortunately, the size of these boundary matrices scales combinatorially with computed homology dimension $k$. For the flag complex of a graph, the number of $k$-cells is the number of $(k-1)$-cliques in the graph. For dense graphs, this number grows combinatorially for increasing $k$ and is at worst $2^n$ for complete graphs on $n$ vertices. Therefore in practice, the computation of persistent homology is generally restricted to the first few dimensions of the complex. We computed persistent homology up to $k = 4$ for many of the knowledge networks, although due to computational limitations, only reached $k = 3$ for some of the larger, denser networks. For the large knowledge networks, persistence computations were run on a node using multiple AMD EPYC 7702 processors and 2TB RAM hosted by the Minnesota Supercomputing Institute.

6.2 Results

6.2.1 Additional Knowledge Networks

To help determine whether the topological dynamics we observe using the USPTO and APS data capture distinctive properties of scientific and technological knowledge production or whether similar dynamics would be observed when tracking the growth of other large, two-mode knowledge networks, we computed persistent homology using data from several Stack Exchange sites. Stack Exchange is a network of question-and-answer websites. While perhaps most famous for Stack Overflow, a programming question-and-answer community, Stack Exchange encompasses a diverse range of topics, from cooking ("Seasoned Advice") and gaming ("Arqade") to server ("ServerFault") and database administration ("Database Administrators"). We focus on five large and representative communities—Mathematics, MathOverflow, Physics, Statistical Analysis, and Theoretical Computer Science—from the set of Stack Exchange sites on science topics. For our purposes, Stack Exchange sites are particularly attractive because, similar to the USPTO and APS data, each community includes a well-defined knowledge categorization system, used to tag questions by topic.

Stack Exchange creates regular snapshots of network websites and makes them freely available for download as database dumps. For our study, we downloaded the snapshot from September 2019, which was the most recent one available at the time of collection. After downloading, we extracted the archives for the five sites of interest. For each site, we then created a two mode edge list, consisting of questions and their associated tags, which was annotated with the date of posting. We subsequently projected this two mode edge list to a one mode representation, after which we were left with a knowledge network consisting of tags that were connected if they appeared together on one or more questions. Similar to our process for the USPTO and APS data, we weight edges based on the number of questions on which the incident tags co-occur. Given the much higher frequency of new questions over time compared to new scientific and technological papers and the much shorter time series (the oldest site in our data, MathOverflow, had been around for only 10 years at the time of data collection), we defined the knowledge networks for the Stack Exchange data on a monthly timescale.

Given this weighted network representation of tags connected by questions, we follow exactly the construction described in Section 2.3, where now $y \in [01/01/2012, 12/01/2019]$ and $c$ is one of the “Mathematics”, “MathOverflow”, “Physics”, “Statistical Analysis”, or “Theoretical Computer Science” sites. We compute the homology of these networks for each site-year combination as was done with the USPTO and APS knowledge
networks (Section 6.1.1). The distribution of Betti numbers over time is presented in Figure S5.

6.2.2 Linguistic Abstraction

To begin, we pulled the full text of abstracts for all patents in our data (abstracts were not available for the APS data at the time of analysis), which we then processed using the Natural Language Toolkit and spaCy Python package. Each abstract was split into a list of tokens, and each token was assigned a part-of-speech tag. Separately for each part of speech (we focus on nouns, verbs, adjectives, and adverbs), tokens were grouped by inflected forms into common lemmas. To allow further grouping, we converted all lemmas (again by part of speech) to lower case, removed extraneous punctuation ('}', '!', '{', '}', ';', ',', '?', '.', '_', '#'), and ensured normalization of white space. For each abstract and part of speech, we then dropped duplicate tokens, so that the resulting data consisted of patent × part of speech × token tuples. We then aggregated these tuples into a balanced subfield × year × part of speech × token panel and counted the number of patents granted in each subfield × year using each part of speech × token in their abstracts. Finally, we joined this panel to our subfield × year data on Betti numbers by dimension.

6.2.3 Comparison to Random Networks

Random graphs play a central role in the study of network complexity, as randomness combined with simple rules of graph construction have been shown to produce complex networks with non-trivial structural features. We were interested in the extent to which the high order structure of knowledge networks may be captured by random graph models and find that, for three popular random graph models, the homological structure of knowledge networks cannot be explained by random models.

We compared the Betti number distribution across five dimensions of the knowledge networks to the Erdős-Rényi (ER) [Erdős and Rényi, 1959], Barabási-Albert (BA) [Barabási and Albert, 1999], and Watts-Strogatz (WS) [Watts and Strogatz, 1998] random graph models. For each knowledge network (each subcategory-year combination), we constructed 10 random graphs with the same number of nodes and approximately equal number of edges (exactly equal for BA and WS models). Because the WS model has two free parameters, we constructed 10 WS graphs across 10 linearly-spaced choices of the rewiring probability parameter in range [0.01, 0.99]. We computed the homology of each randomly-seeded graph and compared the Betti number distributions of the random graphs to the reference knowledge network.

For each dimension and each random network, a one-sample t-test was used to compare the sampled mean Betti numbers of the random model across 10 random seeds to the knowledge network’s Betti number. Of the 1,608 knowledge networks, no random graph model was statistically equivalent in the Betti distribution across all dimensions. Only the Biotechnology subcategory in 2007 was statistically indistinguishable to the WS model in three dimensions (β2, β3, and β4), but these Betti numbers were all trivial. Only 188 knowledge networks contained at least one dimension that was statistically equivalent to a random model with equivalent node and edge distributions. Clearly, the homology of knowledge networks cannot be explained by ER, BA, or WS random models.

Figure S6 shows the distribution of Betti numbers across the random and the knowledge networks. The diagonal depicts a kernel density estimate of the distributions in each dimension while the off-diagonal cells show pairwise cross-sections of Betti numbers. The knowledge networks contain more connected components than the random graph models. In fact, ER is the only model that can produce sizeable graphs with non-trivial β0 (WS can produce disconnected graphs only if the number of nodes is small enough). This difference in β0 is not surprising given BA is constructed by connecting new nodes to a main component and WS assumes full neighborhood connectivity and later re-wires. The most surprising difference between the knowledge and random networks is in the first dimension. The size of β1 in all of the random models is significantly larger than in the corresponding knowledge networks. In short, knowledge networks close 1-dimensional holes at a much higher frequency than would be expected in a randomly distributed model with equivalent node and edge distributions. In the higher dimensions, distributional overlap is closer, but the BA and WS models still show significantly longer tails while the ER model only produces non-trivial β2 and only for dense networks with few nodes.

This comparison to random models shows that the homological structure of knowledge networks cannot be described by simple construction rules. The homology of knowledge networks follows neither a preferential attachment (BA) nor small-world (WS) model. Instead, knowledge networks show a much smoother
distribution of Betti numbers across dimensions wherein the number of holes in each dimension increases up to $\beta_1$ or $\beta_2$ and then decreases in higher dimension. This is in contrast to the BA and WS models which in most parameter combinations show large jumps between $\beta_i$ and $\beta_{i+1}$. As well, the relative lack of 1-dimensional holes in knowledge networks implies some type of higher-order preferential attachment with respect to triplets of knowledge areas in the network. Unpacking this observation offers an exciting route for future investigation.

Figure S1: Knowledge network topology over time at the subfield level. The main plots track counts of Betti numbers, while the inset plots track cell counts. All y-axes are reported on a log scale. The “Physics” panel is highlighted to indicate the different data source (APS) and publication type (academic papers) relative to those of the other panels (where data come from the USPTO and the publication type is patents.)
Figure S2: Collaboration network topology over time at the field level. The main plots track counts of Betti numbers, while the inset plots track cell counts. All y-axes are reported on a log scale. The “Physics” panel is highlighted to indicate the different data source (APS) and publication type (academic papers) relative to those of the other panels (where data come from the USPTO and the publication type is patents). Note that underlying topological features are measured at the subfield level; to generate these field-level plots, we report the average values observed for the constituent subfields. In contrast to approach for knowledge networks (where we use a 1 year window), we define collaboration networks using a 3-year moving window.
Figure S3: Plots of collaboration network topology over time (3 year moving window) Subfield level. The main plots track counts of Betti numbers, while the inset plots track cell counts. All y-axes are reported on a log scale. The “Physics” panel is highlighted to indicate the different data source (APS) and publication type (academic papers) relative to those of the other panels (where data come from the USPTO and the publication type is patents). In contrast to approach for knowledge networks (where we use a 1 year window), we define collaboration networks using a 3-year moving window.
Figure S4: Distribution of average Brysbaert lexical concreteness across homological dimension and part of speech. Concreteness of words used in abstracts within a field falls as high-dimensional Betti numbers increase.

Figure S5: Knowledge network topology over time for Stack Exchange sites (monthly). The main plots track counts of Betti numbers, while the inset plots track cell counts. The main plots track counts of Betti numbers, while the inset plots track cell counts. All y-axes are reported on a log scale.
Figure S6: Distribution differences to topology of random networks. Ten random instantiations of Erdos-Renyi (ER), Barabasi-Albert (BA), and Watts-Strogatz (WS) random graphs were created to match the edge and node distribution for every year of each subcategory of the knowledge network. For the WS model, 10 linearly-spaced values of rewiring value $p$ were chosen for each random initialization, and here only one random initialization is shown for each $p$. The diagonals depict a kernel density estimate for the distributions of the Betti number in each dimension. The off-diagonals depict cross-sections of the distribution across pairs of dimensions.
Table S1: Regressions predicting “hit” publications using lagged topological measures

|                      | Sample: USPTO + APS | Sample: USPTO |
|----------------------|---------------------|---------------|
|                      | (1) (2) (3) (4) (5) | (6) (7) (8) (9) (10) |
| $\beta_0$ (log, t-1)| -0.0119*** -0.0006 -0.0014*** -0.0006 -0.0211*** -0.0056*** -0.0043*** -0.0038*** |
|                      | (0.0003) (0.0004) (0.0004) (0.0004) (0.0004) (0.0005) (0.0005) (0.0005) |
| $\beta_1$ (log, t-1)| -0.0021*** 0.0137*** 0.0104*** 0.0116*** 0.0018*** 0.0100*** 0.0148*** 0.0115*** |
|                      | (0.0003) (0.0004) (0.0004) (0.0004) (0.0005) (0.0005) (0.0005) (0.0005) |
| $\beta_2$ (log, t-1)| 0.0060*** 0.0059*** 0.0055*** 0.0054*** 0.0089*** 0.0058*** 0.0046*** 0.0051*** |
|                      | (0.0001) (0.0002) (0.0002) (0.0002) (0.0001) (0.0002) (0.0002) (0.0002) |
| $\beta_3$ (log, t-1)| 0.0089*** 0.0015*** -0.0003* 0.0027*** 0.0095*** 0.0010*** 0.0003+ 0.0020*** |
|                      | (0.0001) (0.0002) (0.0001) (0.0002) (0.0001) (0.0002) (0.0002) (0.0002) |
| $\Delta_0$ (log, t-1)| 0.0312*** -0.0163*** -0.0067+ 0.0700*** -0.1111*** -0.0731*** |
|                      | (0.0018) (0.0037) (0.0039) (0.0025) (0.0045) (0.0047) |
| $\Delta_1$ (log, t-1)| 0.0865*** 0.0486*** 0.0432*** 0.201*** 0.1879*** 0.1750*** |
|                      | (0.0039) (0.0061) (0.0061) (0.0057) (0.0073) (0.0073) |
| $\Delta_2$ (log, t-1)| -0.2717*** -0.0712*** -0.0690*** -0.2737*** -0.2324*** |
|                      | (0.0051) (0.0061) (0.0062) (0.0078) (0.0085) (0.0085) |
| $\Delta_3$ (log, t-1)| 0.1883*** 0.0284*** 0.0271*** 0.237*** 0.1512*** |
|                      | (0.0035) (0.0038) (0.0040) (0.0059) (0.0061) (0.0061) |
| $\Delta_4$ (log, t-1)| -0.0484*** -0.0015 -0.0016 -0.0702*** -0.0417*** |
|                      | (0.0011) (0.0011) (0.0012) (0.0018) (0.0019) (0.0019) |

Year fixed effects   | No   | Yes  | Yes  | Yes  | Yes  | No   | Yes  | Yes  | Yes  | Yes  |
Field fixed effects  | No   | Yes  | Yes  | Yes  | Yes  | No   | Yes  | Yes  | Yes  | Yes  |
Controls             | Yes  | No   | Yes  | Yes  | Yes  | Yes  | No   | Yes  | Yes  | Yes  |

N                     | 4176784 | 4176784 | 4176784 | 4246553 | 4176784 | 3785961 | 3785961 | 3785961 | 3855730 | 3785961 |
Adjusted R2           | 0.02  | 0.04  | 0.04  | 0.04  | 0.04  | 0.02  | 0.04  | 0.04  | 0.04  | 0.04  |

Notes: Estimates are from ordinary-least-squares regressions (linear probability models). This table evaluates the association between knowledge network topology (measured at the level of the field × year) and the probability of a “hit” publication (patent or paper) using lagged (1 year) topological measures. Hit publications are defined (using a 0/1 indicator variable) as those that are cited more than 95 percent of all other publications across fields and years, as of 5 years after publication. When indicated, included control variables are measures of the number of publications (logged) and knowledge network density for each field × year observation. For more details on variables, see Table 3. Robust standard errors are shown in parentheses; p-values correspond to two-tailed tests.

+p<0.1; *p<0.05; **p<0.01; ***p<0.001