Title:

Science and Technology Advance through Surprise

Short title:

R&D Advance through Surprise

Breakthrough discoveries and inventions involve unexpected combinations of *contents* including problems, methods, and natural entities, and also diverse *contexts* such as journals, subfields, and conferences. Drawing on data from tens of millions of research papers, patents, and researchers, we construct models that predict more than 95% of next year's content and context combinations with embeddings constructed from high-dimensional stochastic block models, where the improbability of new combinations itself predicts up to half of the likelihood that they will gain outsized citations and major awards. Most of these breakthroughs occur when problems from one field are unexpectedly solved by researchers from a distant other. These findings demonstrate the critical role of surprise in advance, and enable evaluation of scientific institutions ranging from education and peer review to awards in supporting it.

19th Century philosopher and scientist Charles Sanders Peirce argued that neither the logics of deduction nor induction alone could characterize the reasoning behind path-breaking new hypotheses in science, but rather their collision through a process he termed abduction. Abduction begins as expectations born of theory or tradition become disrupted by unexpected observations or findings (*1*). Surprise stimulates scientists to forge new claims that make the surprising unsurprising. Here we empirically demonstrate across the biomedical sciences, physical sciences and patented inventions that, following Peirce, surprising hypotheses, findings and insights are the best available predictor of outsized success. But neither Peirce nor anyone since has specified where the stuff of new hypotheses came from. One account is serendipity or making the most of surprising encounters (*2*, *3*), encapsulated in Pasteur's oft-quoted maxim "chance favors only the prepared mind" (*4*), but this poses a paradox. The successful scientific mind must simultaneously know enough within a scientific or technological context to be surprised, and enough outside to imagine why it should not be surprised. Here we show how surprising successes systematically emerge across, rather than within researchers; most commonly when those in one field surprisingly publish problem-solving results to audiences in a distant other. This contrasts with research that focuses on inter- and multi-disciplinarity as sources of advance (*5*–*7*). We show how predictability and surprise in science and technology allow us new tools to evaluate how scientific institutions ranging from graduate education, peer review and awards facilitate advance.

In order to identify the sources of scientific and technological surprise, we must first identify what is expected with precision. Here we follow others in modeling discovery and invention as combinatorial processes linking previous ideas, phenomena and technologies (*8*–*12*). We separate combinations of scientific contents and contexts in order to refine our expectations about normal scientific and technological developments in the future (*13*). A new scientific or technological configuration of contents—phenomena, concepts, and methods—may surprise because it has never succeeded before, despite having been considered and attempted. A new configuration of contents that cuts across divergent contexts—journals and conferences—may surprise because it has never been imagined. The separate consideration of content and contexts allows us to contrast scientific discovery and technological search: Fields and their boundaries are clear and ever-present for scientists at all phases of scientific production, publishing and promotion, but largely invisible for technological invention and its certification in legally protected patents.

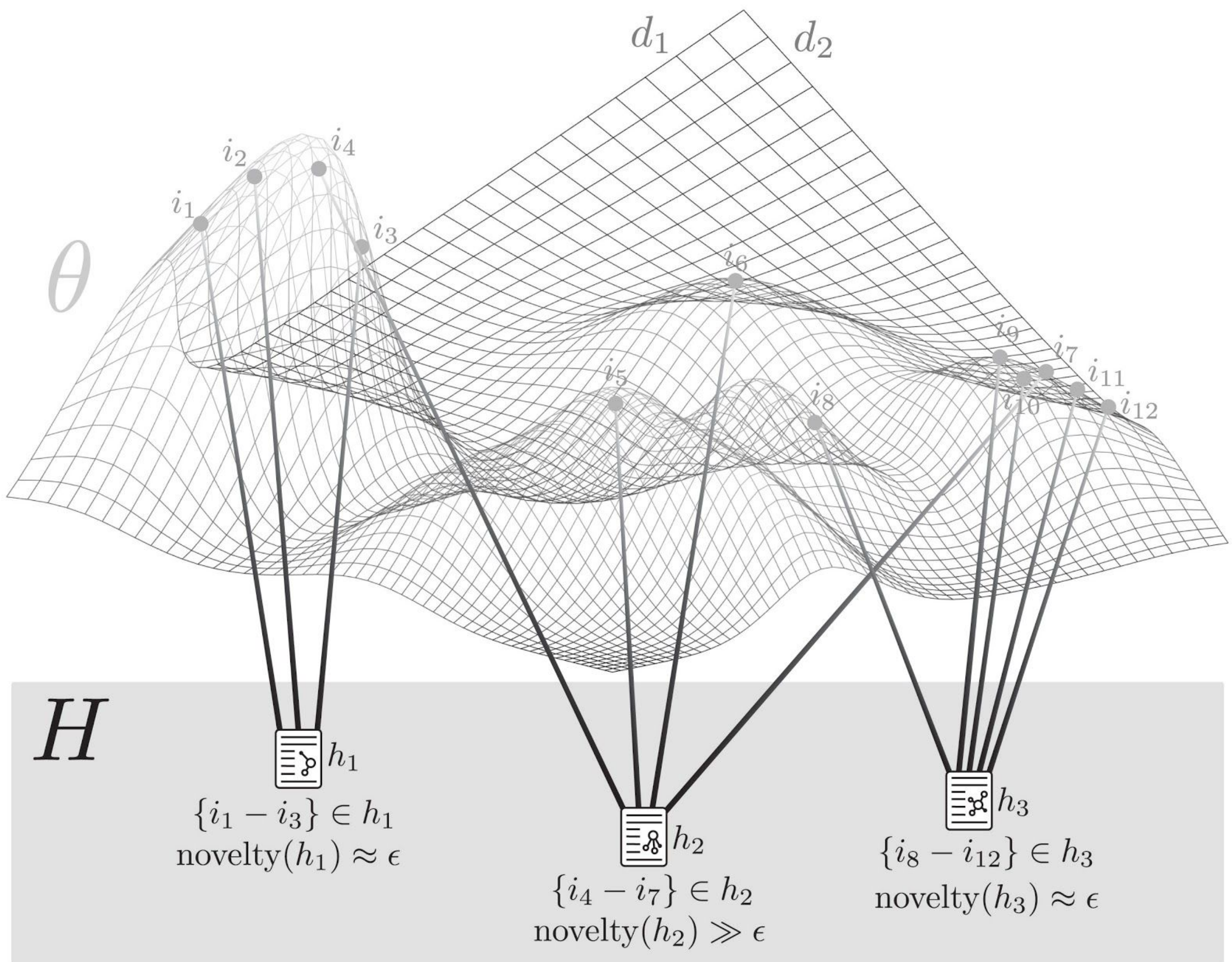
Virtually all empirical research examining combinatorial discovery and invention has deconstructed new products into collections of pairwise combinations (*11*), resting on mature analysis tools for simple graphs that define links between entity pairs. Recent research, however, has demonstrated the critical importance of higher-order structure in understanding complex networks, ranging from the hub structure of global transportation networks to clustering in neuronal networks (*14*) to stabilizing interaction between species (*15*, *16*). Here we develop a method to model the frontiers of science and technology as a complex hypergraph drawn from an embedding of contents and contexts (*17*) using mixed-membership, high-dimensional stochastic block models, where each discovery or invention can be rendered as a complete set of scientific contents and contexts. We demonstrate that adding this higher-order structure both improves our prediction of new articles and patents and those that achieve outsized success.

In this study, we apply our framework to three major corpora of scientific knowledge and technological advance: 19,916,562 biomedical articles published between 1865 - 2009 from the MEDLINE database; 541,448 articles published between 1893 - 2013 in the physical sciences from journals published by the American Physical Society (APS), and 6,488,262 patents granted between 1979 - 2017 from the US Patent database (see SM Data Description for details). The building blocks of content for those articles and patents are identified using community-curated ontologies—Medical Subject Heading (MeSH) terms for MEDLINE, Physics and Astronomy Classification Scheme (PACS) codes for APS, and USPTO technology subclass codes for patents. Then we build embeddings for each dataset in each year, and a corresponding hypergraph where each node represents a code from the ontologies and each hyperedge corresponds to a paper or patent that inscribes a combination of those nodes.

We build corresponding embeddings and hypergraphs of context where nodes represent journals, conferences, and major technological areas (for patents) that scientists and inventors draw upon in generating new work. Each hyperedge corresponds to a paper or patent that incribes a combination of context nodes cited in their references. To predict new combinations, we develop a generative model that extends the degree-corrected stochastic block model into high-dimensions, probabilistically characterizing common patterns of complete combinations. We model the likelihood that contents or contexts become combined as a function of their (1) *complementarity* in a latent scientific space and (2) cognitive *availability* to scientists through prior usage frequency. Specifically, each node i is associated with a latent vector θ_i that embeds the node in a latent space constructed to optimize the likelihood of the observed papers and patents. Each entry θ_{id} of the latent vector denotes the probability that node *i* belongs to a latent dimension *d*. The complementarity between contents or contexts in a combination *h* is modeled as the probability that those nodes belong to the same dimension, $\sum_d \prod_{i \in h} \theta_{id}$. We account for each content's and context's cognitive availability as most empirical networks display great heterogeneity in node connectivity, with few contents and contexts intensively drawn upon in many papers and patents. Accordingly, we associate each node i with a latent scalar r_i to account for its cognitive availability or the exposure scientists have had to it, capturing its overall connectivity in the network. The propensity (λ_h) of a combination h—our expectation of its appearance in actual papers and patents—is then modeled as the product of the complementarity between the nodes in h and their availabilities:

$$\lambda_h = \sum_d \prod_{i \in h} \theta_{id} \times \prod_{i \in h} r_i \ .$$

Then the number of publications or patents that realize combination *h* is modeled as a Poisson random variable with λ_h as its mean. Finally, the likelihood of a hypergraph G is the product of the likelihood of observing every possible combination (see SM for details).



$$\text{novelty}(h) = -\log \sum_{d} \prod_{i \in h} \theta_{id}$$

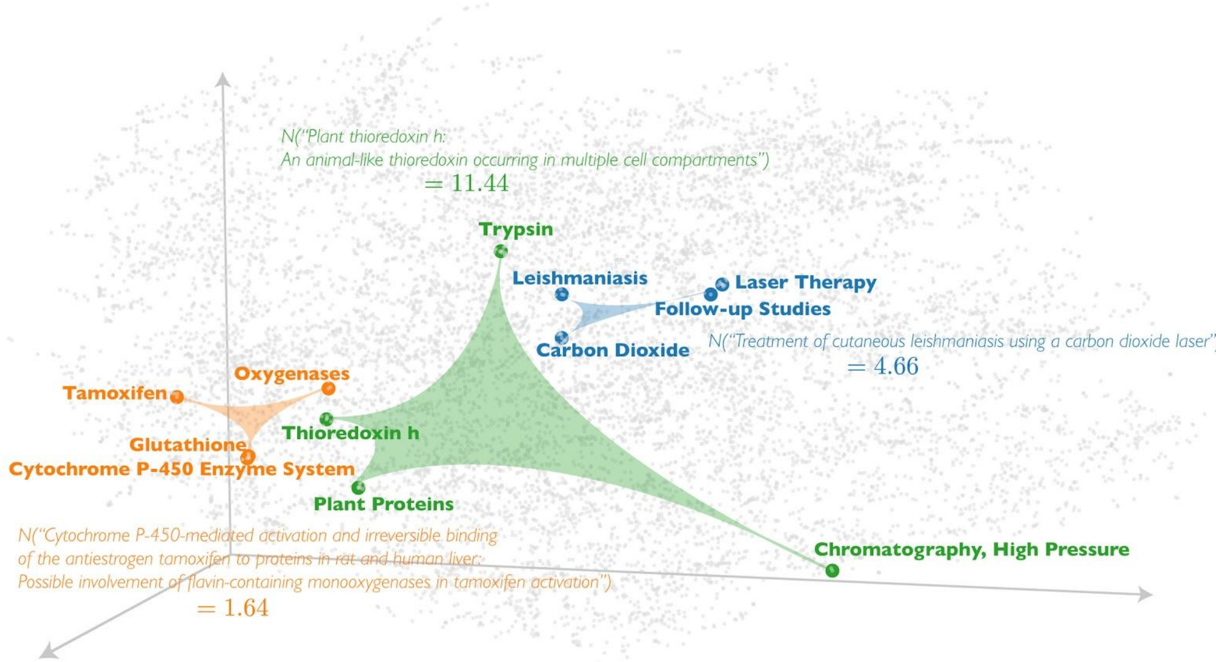


Figure 1. (Top) Illustration of the manifold inscribing all topics θ and an evaluation of three articles or patents (hyperedges $h_{1\text{-}3}$) in terms of their novel combinations. Articles/patents h_1 and h_3 represent projects that combine scientific or technical components near one another in θ, making each of high probability and low (ε) novelty—similar to many related papers from the past. By contrast, paper h_2 draws a novel combination of components unlike any paper from the past, making it of low probability and high ($\gg \varepsilon$) novelty. **(Bottom)** Actual three dimensional projection of the manifold best inscribing all MeSH codes from MEDLINE articles in our analysis. Also included are MeSH terms in the most novel article (blue), the least novel article (orange), and a random article in between (green) among all articles including four MeSH terms.

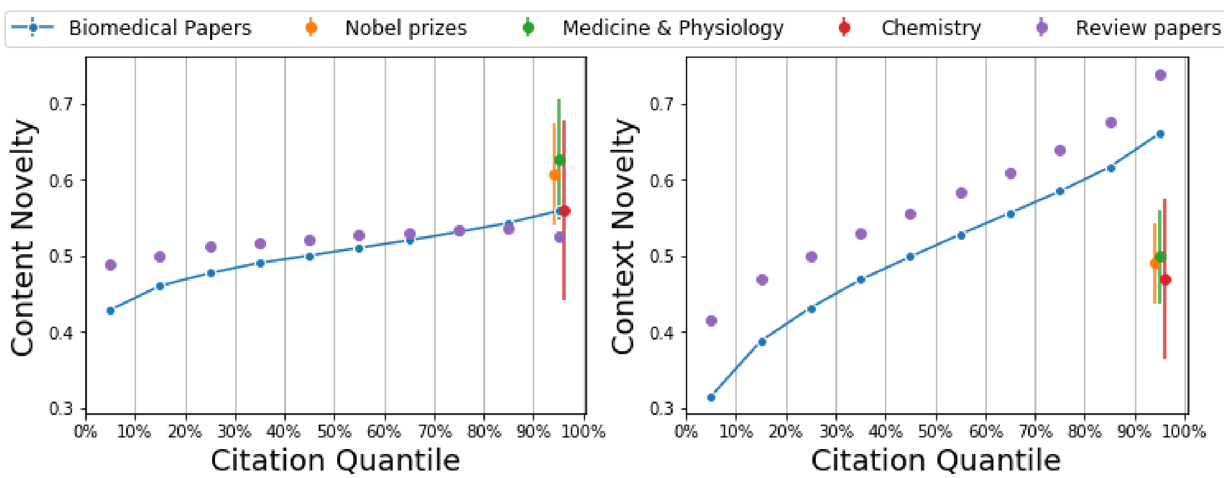
Across the biomedical sciences, physical sciences, and inventions, the model correctly distinguishes between a content combination that turned into a publication and a random combination more than 95% of the time based on data from previous years (Biology: AUC=0.98; Physics: AUC=0.97; Inventions: AUC=0.95) (See SM for details). New context combinations are also predictable (Biology: AUC=0.99; Physics: AUC=0.88; Inventions: AUC=0.83). The model implies that researchers tend to conservatively wander locally across the latent knowledge space constructed from papers and patents in prior years to arrive at those published the following year. This agrees with previous findings on the inertia in scientific and technological investigations as teams wander locally across contents and contexts to extend their own and colleagues' prior work (*18*).

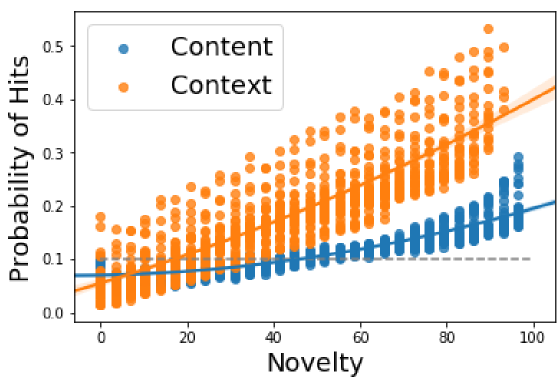
With a measure of what science and technology is common and expected, we assess surprising, improbable combinations as the inverse likelihood or surprisal of *h* (*19*, section 3.3):

$$novelty(h) = -\log \sum_{d} \prod_{i \in h} \theta_{id} . \qquad (2)$$

We examine how novelty is associated with publication citation impact and awards by dividing MEDLINE papers into 10 equal-sized groups based on citation counts, i.e., the first group contains the least 10% cited papers, the second group the next 10%, and so on. Both content and context novelties increase significantly with citation quantiles, as shown in Figure 2 (Top). Further, we show that Nobel prize-winning papers, which are in the top 10% citation group, have average context novelty, but extreme content novelty. This divergence between citations and awards is likely because citations are conferred by everyone who benefits from an advance, but awards are provided by a particular scientific community or context, which apparently undervalues breakthrough advances that transgress established boundaries (*20*).

Moreover, the probability of being a hit paper—in the top 10% of most cited papers published in the same year—also increases monotonically with the rank of novelty. For MEDLINE papers, those with the most novel combinations of context are 3.5 times more likely to be a hit paper than random, and novel content combinations are 2 times more likely, and a novel joint combination is 4.5 times more likely. Articles with maximal context and content surprise predict nearly 50% of the likelihood of being in the top 10% of citations.




Content
Context
Probability of Hits
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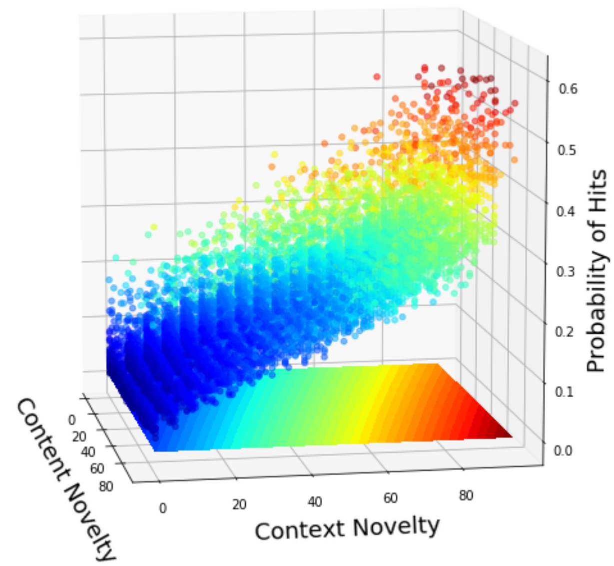
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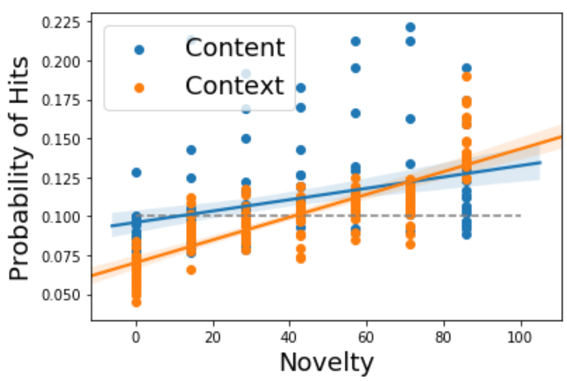
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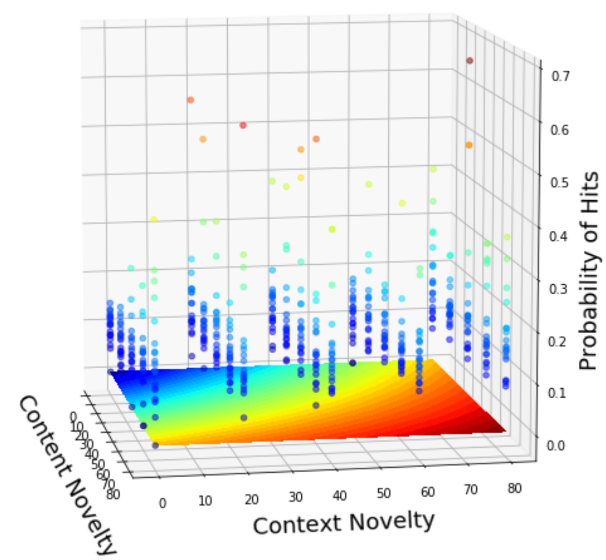
Content Novelty
Context Novelty
Probability of Hits

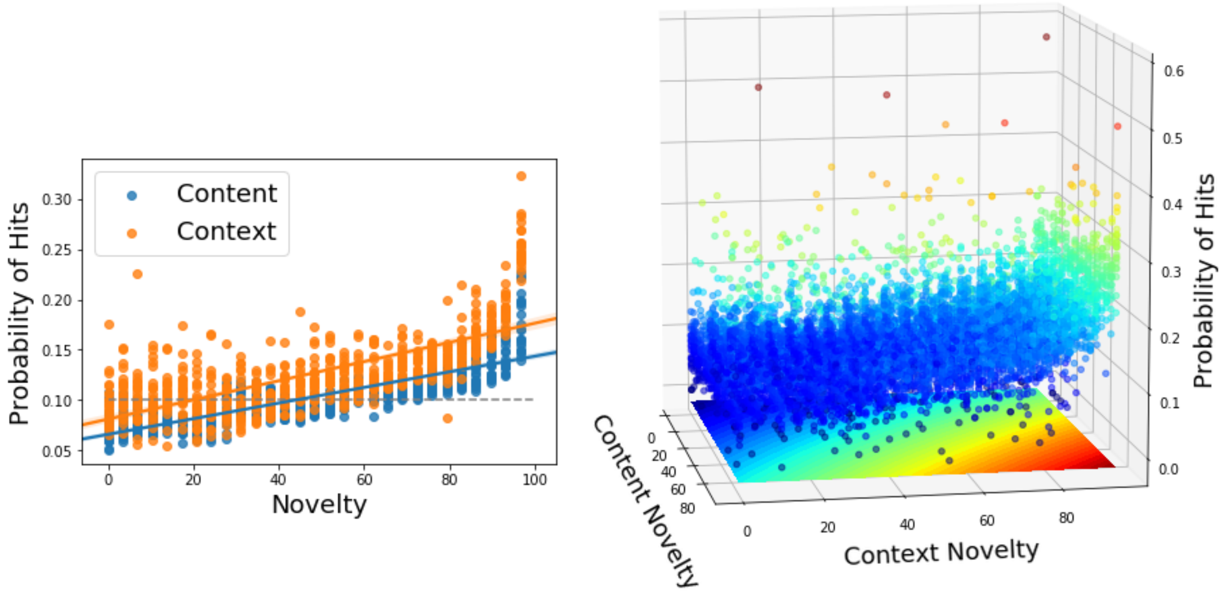

Figure 2: Average content and context novelty for each decile of citations, tracing a monotonic rise; Including average for Nobel prizes in Physiology or Medicine, Chemistry (first row). Probability of being a hit paper as a function of content and context novelty separately (row 3-5, left) and jointly (row 3-5, right). Third row shows results for MEDLINE data, fourth row for APS data, and bottom row for the USPTO data. For each, bivariate distribution of content and context novelty across articles or patents on the left.

Unlike the biomedical papers, novel patents are only 2 times more likely to be a hit patent than random. Disciplinary boundaries are weaker in the technology space, where patent examiners, unlike scientific reviewers, do not enforce them. The lack of discrete fields enables technologists to search more widely, but reduces the signal from violations of context in the prediction of advance.

Both content and context combinations are good predictors of impact, by they provide nearly independent information regarding the ongoing construction of scientific ideas and technological artifacts. The correlation between propensities for content and context combinations are extremely low across biomedicine (0.01), physics (0.05), and inventions (0.03). When we calculate the content similarity between cited papers and the publishing venues in which they are published, we see that scientists cite content from contexts familiar to those venues 500% more intensively than content from contexts that are distant (*23*). Inventors of patented technologies, however, are not reviewed by peers and cite close or distant sources with roughly the same probability (Figure 1 left and Supplementary Materials). Following from this difference, we find that the distribution of collective attention differs dramatically in science versus technology. We quantify the spread of attention with the normalized entropy of the number of publications containing each content node, shown in Figure 1 right. Content nodes in the patent space receive much more equal attention (higher entropy), compared to MEDLINE or APS.

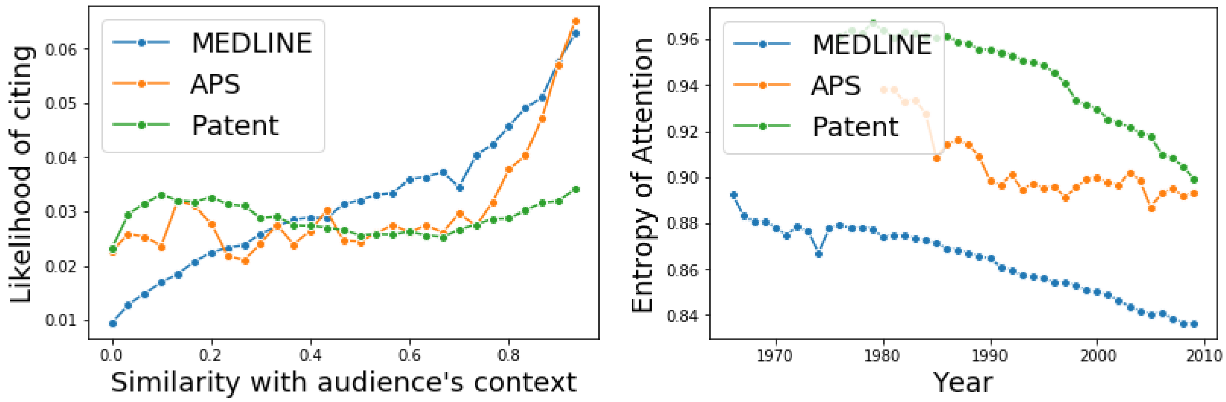

Figure 3: Left: The likelihood of citing context nodes variously familiar within the publication venue for papers in MEDLINE (blue curve), APS (orange curve), and US Patent (green curve). Papers in MEDLINE and APS reference contexts similar to those in which they are published much more intensively than contexts that are distant. Patents, by contrast, reference close or distant sources with roughly the same likelihood. Right: Entropy of attention on the content nodes over time. The entropy of attention is calculated as the entropy of the number of publications associated with each content node. To compare entropy across datasets, it is normalized by the logarithm of the number of content nodes in each dataset. The content nodes in the patent space receive more equal attention (higher entropy), compared to MEDLINE and APS, across the years shown in the figure.

Finally, we explore the relationship between scientists' backgrounds and breakthrough. Do unusual individual scientist backgrounds, atypical collaborations, or unexpected expeditions where scientists and inventors reach across disciplines and address problems held by a distant audience contribute most to novelty and impact? Using context (e.g., journals, conferences) embeddings, θ_i, and Eq. 2, we quantify the (1) *career novelty* of a scientist by the surprisal of the combination of contexts she has ever published, (2) *team novelty* by the combination of contexts brought together across team members' publication histories, and (3) *expedition novelty* by the average distance between the backgrounds of team members and their audience formalized by their publication venue. Figure 4 (left) shows that the probability of being a hit paper increases gradually with career and team novelty, but expedition novelty rises much more quickly as the strongest predictor. Papers involving the most unexpected publication events or conversations are 3.5 times more likely than random to be hit papers. Figure 4 (left) also shows that career and team novelties are highly correlated, suggesting that successful teams not only have members from multiple disciplines, but also members with diverse backgrounds who "glue" interdisciplinary teams together (also see Figure S3). Successful knowledge expeditions, however, are the most likely path associated with breakthrough discovery. When regressing content and context novelties of a paper separately on the three background novelty measures, we find that expedition novelty has by far the largest effect on context novelty ($\beta = 2.23,\ p < .001$), but team novelty has the marginal top effect on content novelty ($\beta = 0.75,\ p < .001$).

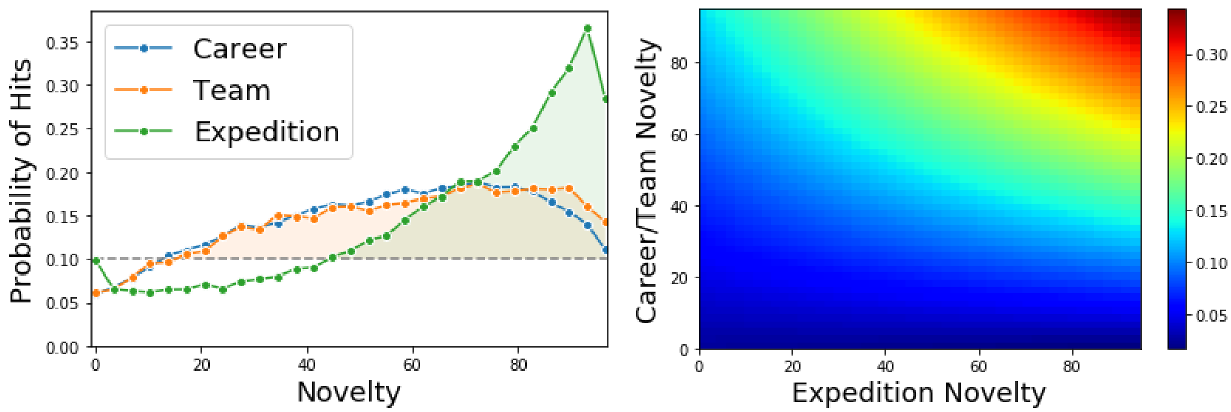

Figure 4: Left: The probability that a hit biomedical paper was produced by scientists manifesting greater career, team and expedition novelty; with career and team novelty closely correlated and expedition novelty sharply deviating. Right: Taking the average of Career and Team Novelty on the y-axis and Expedition novelty on the x-axis, we see the critical interaction between these novel exposures and generating discoveries that garner outsized attention.

In this paper we demonstrate the striking predictability of future scientific articles and technology patents, which results from a system in which researchers, their collaborators, students, and fields produce self-similar streams of research over time. We then justify the importance of surprise in unfolding discovery and invention, revealing that up to 50% of outsized success (in biomedicine) can be predicted by improbability under models that predict new research products. Most of those unpredictable successes occurred not necessarily through interdisciplinary careers or multi-disciplinary teams, but from scientists in one domain solving problems in a distant other. This implies the operation of collective abduction, where violations of theoretical and traditional expectations drive collective attention. It further suggests the cross-disciplinary search process by which problems, puzzles and conflicts in one area of science become discovered by scientists in other areas whose exposure to foreign theories and findings enable them to make surprising discoveries.

We also technically demonstrate that prediction of complex content and context bundles dramatically benefit from taking into account the high-dimensional structure of complete combinations, rather than viewing them as sets of pairwise combinations. This suggests the potential importance of representing high-dimensional structure like sets in a form that captures their native complexity for characterization and prediction.

Our findings suggest how models that predict normal and outsized advance represent powerful tools for evaluating the degree to which scientific and technical institutions facilitate progress. For example, our work shows that granting scientific awards for breakthrough progress, from Nobel Prizes to the plaques and certificates sponsored by nearly every scientific society are biased towards some forms of surprise and away from others. Scientific societies convene conferences and publish journals, the central contexts that showcase new findings, and so it is notable that they tend to award surprising combinations of scientific contents but not contexts, but that novel context combination are most predictive of outsized citations and scientific importance. This suggests that awards, as currently offered, represent a conservative influence on scientific advance (*20*). Similarly, our findings reveal that scientists amplify the familiarity of their work to colleagues, editors and reviewers, increasing their citation of familiar sources by nearly 500%, likely in order to appear to build on the shoulders of their audience. This reinforces the internal focus of dense fields, which collectively learn more about less. Inventors, by contrast, cite and search widely to know less about more (*24*), providing new evidence for complementarities between search in science and technology and justifying why fundamental insights emerge not only from fundamental investigations, but also practical ones (*25*–*27*). Finally, our work has implications for graduate education. Novel careers, novel combinations of experience within teams, but most critically, researchers seeking out problems and subjects held by distant audiences, if successful, dramatically increase the likelihood that their work will disrupt scientific attention with insights received as path breaking. This suggests that education seeking to cultivate scientific breakthroughs might teach trans-disciplinary search for problems, and frame every student, team and expedition as an experiment, whose complex combination of background experiences could condition novel hypotheses with the potential not only to succeed or fail, but to radically alter science.

Supplementary Materials

Data Description

This work investigated three major corpora of scientific and technological knowledge: 19,916,562 papers published between 1865 - 2009 in biomedical sciences from the MEDLINE database, 541,448 papers published between 1893 - 2013 in physical sciences from all journals published by the American Physical Society, and 6,488,262 patents granted between 1979 - 2017 from the US Patent database. The building blocks of content for those articles and patents are identified using community-curated ontologies—Medical Subject Heading (MeSH) terms for MEDLINE, the Physics and Astronomy Classification Scheme (PACS) codes for APS, and technology subclass codes for patents. Then we build hypergraphs of content where each node represents a code from the ontologies and each (hyper)edge corresponds to a paper or patent that embodies a combination of the nodes.

MEDLINE

MEDLINE is the U.S. National Library of Medicine's bibliographic database. It contains abstracts, citations, and other metadata for more than 25 million journal articles in biomedicine and health, broadly defined to encompass those areas of the life sciences, behavioral sciences, chemical sciences, and bioengineering. The version of data used in this study contains 19,916,562 papers published between 1865 - 2009. Because the coverage for papers prior to 1966 is somewhat limited, our analysis focuses on papers published in and after 1966, but with the pre-1966 papers as background information when predicting new content and context combinations and their novelty.

Medical Subject Headings (MeSH) is the National Library of Medicine's (NLM's) controlled terminology used for indexing articles in MEDLINE. It is designed to facilitate the determination of subject content in the biomedical literature. MeSH terms are organized hierarchically as a tree with the top level terms (called headings) corresponding to major branches such as "Diseases" and "Chemicals and Drugs", with multiple levels under each branch. Terms in the bottom level are the most fine-grained, detailed concepts associated with distinct biological phenomena, chemicals, and methods. We use the bottom-level terms from the 3 branches that are central to the biomedical field - "Diseases", "Chemicals and Drugs", and "Analytical, Diagnostic and Therapeutic Techniques and Equipment" - as nodes in the hypergraphs of content of MEDLINE papers. Terms from the Diseases branch include conditions such as "lathyrism" and "endometriosis"; examples from the Chemicals and Drugs branch include "elastin", "tropoelastin", "aminocaproates", "aminocaproic acids", "amino acids", "aminoacetonitrile", and "amyloid beta-protein"; and examples from the Analytical, Diagnostic and Therapeutic Techniques and Equipment branch (or methods for short) include "polyacrylamide gel electrophoresis", "ion exchange chromatography", and "ultracentrifugation". NLM curators manually affix MeSH codes to papers as they are ingested into MEDLINE and made available through its popular PubMed database.

APS

The APS dataset is provided by the American Physical Society (APS). It contains 541,448 papers published between 1893 and 2013 in 12 physics journals: *Physical Review*, *Physical Review A*, *B, C, D, E, I* and *X*, *Physical Review Special Topics - Acceler and Physics*, *Physical Review Letters*, and *Reviews of Modern Physics*.

The dataset contains basic metadata for each paper including title, publication year, abstract, etc. It also contains the PACS (Physics and Astronomy Classification Scheme) codes associated with each paper. We use the PACS codes as nodes in hypergraphs of content to characterize APS papers. The Physics and Astronomy Classification Scheme was developed by the American Institute of Physics in 1970 and has been used by APS since 1975, although the AIP is currently developing a new research thesaurus to replace PACS, due to the complexity and expense involved in the update of PACS. Similar to MeSH terms, PACS is also a hierarchical partition of the whole spectrum of subject matter in physics, astronomy, and related sciences. Because PACS codes are not available for papers published before 1975, our analysis focuses on APS papers published in and after 1975. Like MeSH, PACS codes are arranged hierarchically, and include "Mathematical methods in physics", which range from "Quantum Monte Carlo Methods" to "Fourier analysis"; "Instruments…" such as "Electron and ion spectrometers" and "X-ray microscopes"; "Specific theories…" like "Quark-gluon plasma" and "Chiral Langrangians"; and "...specific particles" ranging from "Baryons" to "Quarks". Unlike MeSH codes, which are added by curators, authors affix PACS codes to their own papers through the publishing process.

The dataset only contains citations between the APS papers. In order to obtain external citations we query the Web of Science (WOS) database to collect all the journals cited by the APS papers. Particularly, in the WOS database we find all the papers published by the 12 APS journals, and then all the journals cited by those papers. The journals are then used as nodes in hypergraphs of context for the APS papers. Additionally, we also query the WOS database to collect the number of citations a paper receives for more accurate assessment of the papers' impact.

US Patent

The US Patent dataset is released by the US Patent & Trademark Office (USPTO). It contains 6,488,262 patents published between 1979 and 2017. The dataset contains basic metadata for each patent such as title, publication year, USPC (United States Patent Classification) codes, etc. The USPC is a classification system used by USPTO to organize all U.S. patent documents and other technical documents into specific technology groupings based on common subject matter. The USPC is a two-layer classification system. The top layer consists of terms called classes, and each class contains subcomponents called subclasses. According to USPTO, a class generally delineates one technology from another and every patent is assigned a main class. As such, we use the class codes as nodes in the hypergraphs of context for patents.

Subclasses delineate processes, structural features, and functional features of the subject matter encompassed within the scope of a class, and thus we use subclass codes as content nodes for the patents. In total, there are 158,073 subclass codes (content nodes) and 496 class codes (context nodes).

On January 1, 2013, the USPTO moved to a new classification system called the Cooperative Patent Classification (CPC); consequently, our analysis is restricted to patents granted before 2013.

Nobel Prize Papers

The Nobel prize-winning papers are derived from the Nobel laureates dataset by Li et al. (*29*), which contains publication histories of nearly all Nobel prize winners from the past century. However, their focus is on the Nobel laureates, but ours is on award-winning papers. While it is relatively easy to find out the person who won a prize, it is hard to pinpoint the papers that contribute to the winning of the prize. Li et al. take a generous approach by including papers cited by Nobel lectures and papers published in the same period of one's prize-winning work (while satisfying several inclusion criteria; see (*29*) for details). This results in some noises for our analysis as not every paper in their dataset is a prize-winning paper. As a conservative solution, for every Nobel laureate we take the most cited paper in the dataset as the award-winning paper and use only those papers as award-winning papers in our analysis. We acknowledge that a Nobel prize could be attributed to a series of work and this filtering process might miss a few papers, but the most important (in terms of impact) paper for every prize is kept and every paper remaining is most likely an award-winning paper.

Method

Higher-Order Stochastic Block Model

For a given hypergraph, whether comprised of content or context nodes, the propensity of any combination of nodes to form a hyperedge is modeled as a product of two factors: the complementarity between the nodes in the combination and their cognitive availabilities. Combinations with higher propensity will be more likely to turn into papers and patents, agreeing with the intuition that people tend to search locally and pursue trending topics.

To formulate this idea formally, each node i is associated with a latent vector θ_i that positions the node in a latent space constructed to optimize the likelihood of observed papers and patents. Each entry θ_{id} of the latent vector denotes the probability that node *i* belongs to a latent dimension *d*, and thus $\sum_{d=1}^{D} \theta_{id} = 1$. The complementarity between nodes in a combination *h* is modeled as the probability that those nodes belong to the same dimension, $\sum_{d} \prod_{i \in h} \theta_{id}$. This formulation represents an extension of the mixed-membership stochastic block model in (*30*), which was designed for networks with only pairwise interactions.

We also account for each node's cognitive availability because most empirical networks display great heterogeneity in node connectivity, with few contents intensively drawn upon and few contexts widely attended or appreciated across many papers and patents. Previous work (*31*) has shown that by integrating heterogeneity of node connectivity, the performance of community detection in real-world networks dramatically improves. Accordingly, we associate each node i with a latent scalar r_i to account for its cognitive availability, presumably associated with its overall connectivity in the network.

Assembling these components, the propensity (λ_h) of combination h—our expectation of its appearance in actual papers and patents—is modeled as the product of the complementarity between the nodes in h and their availabilities

$$\lambda_h = \sum_{d} \prod_{i \in h} \theta_{id} \times \prod_{i \in h} r_i \, . \tag{1}$$

To link the propensities to their observed appearances, we model the number of papers or patents X_h that embody a certain combination h as a Poisson random variable with the propensity of that combination as its mean:

$$X_h \sim Poisson(\lambda_h)$$

Accordingly, the probability of observing a hypergraph G is the product of probabilities of observing all possible combinations:

$$P(G|\Theta, R) = \prod_{h \in H} P(x_h|\Theta, R) \, ,$$

where x_h is the number of observed papers or patents that realize combination h and H is the set of all possible combinations. (Θ, R) denotes all unknown parameters: $\Theta = (\theta_1, \ldots, \theta_n)$ and $R = (r_1, \ldots, r_n)$.

Finally, we model a time sequence of hypergraphs $(G^1, \ldots, G^T)$ as the output of a Hidden Markov Process on latent parameters Θ, R:

$$P(G^1, \ldots, G^T|\Theta^1, .., \Theta^T, R^1, \ldots, R^T) = P(G^1|\Theta^1, R^1) \prod_{t=2}^{T} P(\Theta^t, R^t|\Theta^{t-1}, R^{t-1}) P(G^t|\Theta^t, R^t) \, ,$$

where time is indexed by the superscript t.

Given articles published by a certain year T, we estimate parameters $(\Theta^1, \ldots, \Theta^T, R^1, \ldots, R^T)$ by maximizing the likelihood function above via stochastic gradient descent. Then the model enables us to predict combinations in year $T+1$. However, even with stochastic gradient descent, model estimation is still computationally challenging due to the vast space of possible combinations. We address these issues in the estimation process as follows. First, the space of possible combinations is exponentially large (on the order of 2^n), and it is computationally prohibitive to go over all possible combinations even with stochastic gradient descent. However, it is extremely rare for large combinations to turn into hyperedges, and hence, we restrict the set of possible combinations to include only combinations no larger than the largest hyperedge observed. Second, since the real hypergraphs are sparse, the sets of hyperedges and non-hyperedge combinations are exceedingly unbalanced with the number of hyperedges to be on the order of n but the number of non-hyperedge combinations on the order of n^D (where D is the size of the largest hyperedge after reducing the space of possible combinations). We employ a widely used approach, negative sampling, in machine learning to address this unbalance issue. Specifically, in each iteration of the training (optimization) process, we randomly sample as many non-hyperedge combinations as the hyperedges to construct balanced hyperedge and non-hyperedge sets. Lastly, to facilitate the stochastic gradient descent, we take a mini-batch of hyperedges and non-hyperedges to compute the gradient of the objective function at each step of the training process.

Model Evaluation

As a brief summary, we study 3 datasets: MEDLINE, APS, and US Patent; each dataset contains hypergraph data over several decades; and we model content and context hypergraphs separately. Consequently, we estimate hundreds of models with each model fitted to a specific hypergraph (content or context) from one of the three datasets up to a certain year. Then, we evaluate the fitness of each model by its predictive performance of (out-of-sample) future combinations.

For example, given hypergraphs of MeSH terms up to and including year 2008, we estimate the stochastic block model, and use the estimated model to predict hyperedges in 2009. Specifically, using the estimates of the parameters (θ, r) for year 2008, we compute the propensity λ_h of any combination h of MeSH terms in year 2009, following Equation (1) $\lambda_h = \sum_c \prod_{i \in h} \theta_{ic} \times \prod_{i \in h} r_i$. Then we assess the model's predictive performance in terms of its AUC (Area Under the Operator-Receiver Curve). Statistically speaking, AUC is the probability that a random combination which turned into a hyperedge (positive combination) in 2009 have a larger propensity than a random combination that did not turn into a hyperedge (negative combination) in 2009. To estimate this quantity, we randomly sample a positive combination and a negative combination from 2009, and check whether the positive combination has a larger propensity than the negative. The simulation is repeated for 10000 times and we calculate the fraction of times where the positive has larger propensity than the negative, which is our estimation of the AUC score in predicting hyperedges in 2009. It is easy to see that a perfect predictor would achieve an AUC score of 1 and random guesses would have an AUC of around 0.5. The larger the number, the better the predictive performance.

Preference on context citations

To assess the extent to which scientists and inventors cite contexts (e.g., journals and conferences) that are familiar to their audience, we compute the similarity between every pair of context nodes where one cites the other. For example, for a paper *i* published in journal *X*, we calculate the similarity between the journal *X* and every journal cited by paper *i.* The similarity is quantified by the cosine similarity between two vectors representing the content of the two journals, conditioned on the content of paper *i*. Specifically, each journal is represented by a vector and each entry in the vector corresponds to a content node (MeSH terms, PACS codes, or subclasses); the value of an entry is the number of papers containing the corresponding content node and ever published by the journal, appropriately normalized so that the sum of the vector is 1. In other words, the vector consists of the loadings of the journal on different contents. When calculating the similarity between two journals, we don't directly compute the cosine similarity between their vectors, as the vectors contain a lot of information irrelevant to the paper currently under consideration. Instead, we only use the entries corresponding to the content nodes in paper *i* to calculate the cosine similarity between the two journals.

As we sweep through all the papers (or patents), a distribution of the similarity between citing-citee context pairs is obtained: the number of times for which context nodes at a given similarity with the audience context (i.e., the citing context) are cited. To appropriately normalize this distribution, we also compute the potential space of citation similarity, which is the number of times for which context nodes at a given similarity would be cited at random. This is achieved by the following procedure: for each paper, sample as many context nodes uniformly at random from all the context nodes as those originally cited, treat the sampled context nodes as if they were cited by the paper, and carry out the same similarity calculations as above. Finally, we have two distributions of similarity between citing-citee context pairs - one observed and one simulated by random sampling - and we take the ratio of the two as the likelihood of citing a context at a given similarity with the audience's context.

<u>Supplementary Results</u>

Density plot of content embeddings

As an illustration of the embedding space, we take all the MeSH terms that are active in 1990 (associated with any paper published in 1990) and project their high-dimension embeddings onto the 2D plane using t-SNE; a Gaussian kernel density is then fit to the 2D points of the nodes (Figure S1).

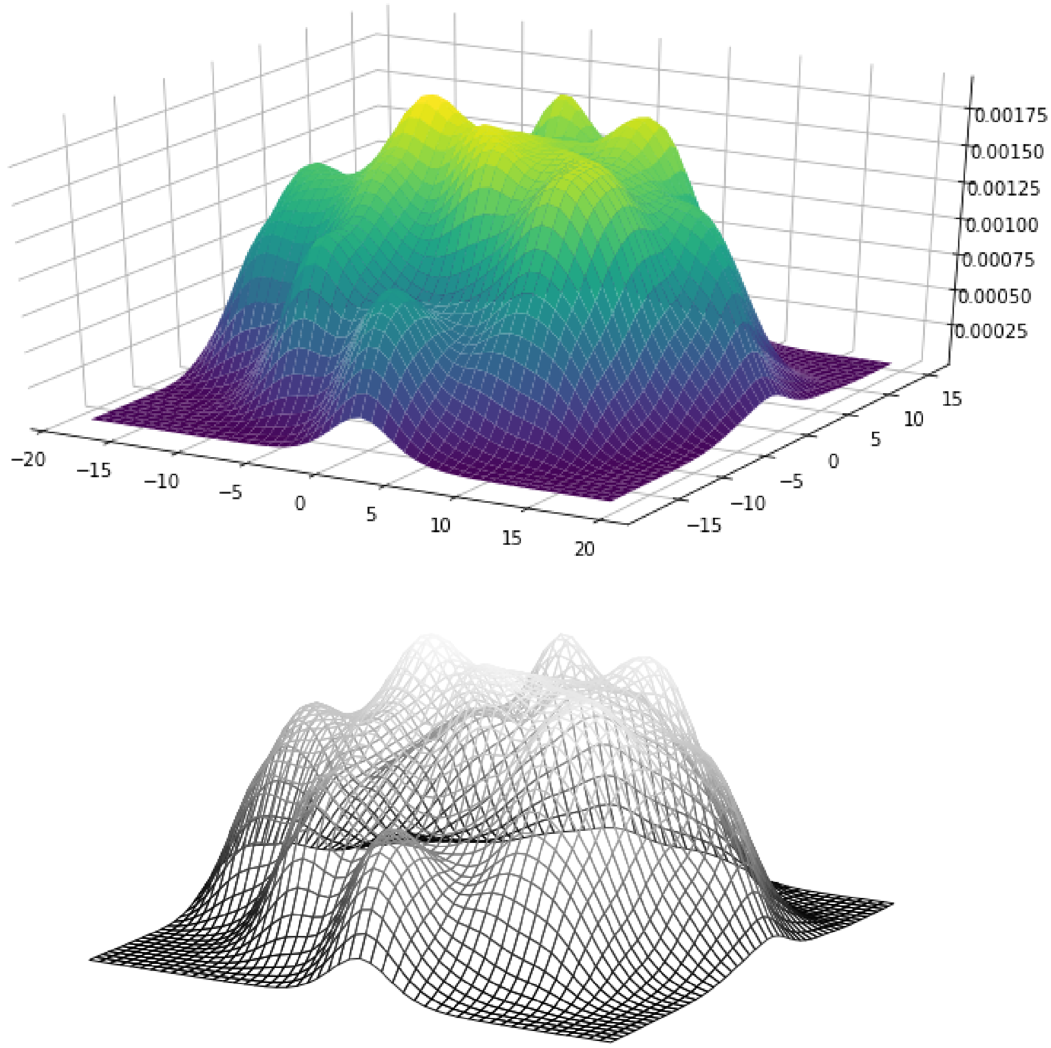

Figure S1. Density plot of 2D projections of the MeSH terms in papers published in 1990.

Novelty and impact for APS papers

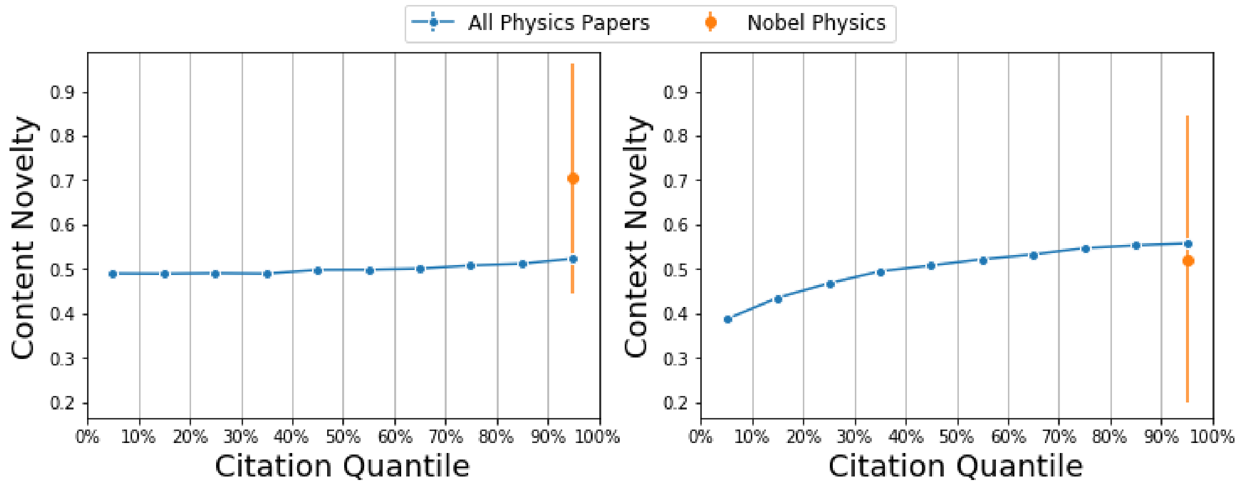

Figure S2: Average content and context novelty for each decile of citations, tracing a monotonic rise; Including average for Nobel prizes in Physics.

Joint Impact of team and career novelty

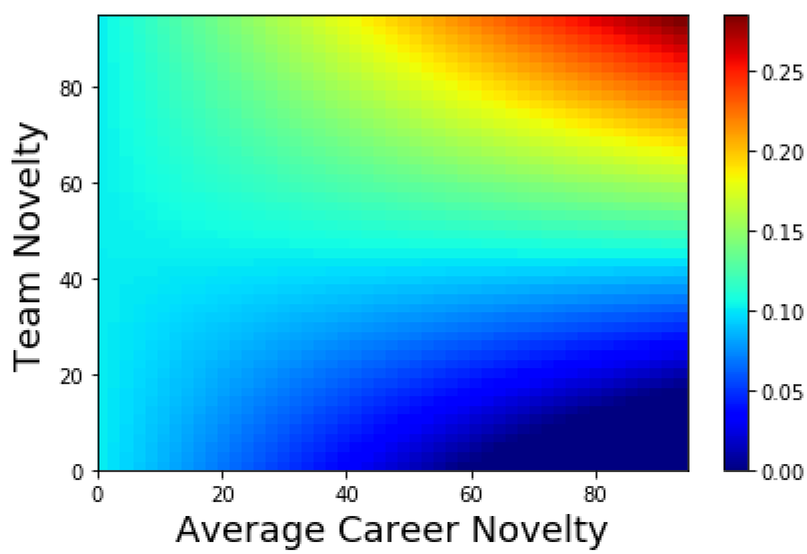

Figure S3. Joint impact of team and career novelty on the probability of being a hit paper. Average career novelty denotes the average of team members' individual career novelty.

<u>Limitations</u>

Our study provides recommendations for improving search in science and technology, but not designs for a machine that generates surprising future discoveries and inventions, because our model only predicts how surprising combinations that *succeed* at publication become success. A vast range of content, context, and background combinations that are nonsensical or doomed, if systematically pursued in a self-conscious search for surprise, would dramatically decrease the rate of outsized success we demonstrate here. Our high-dimensional treasure map does not show where X marks the spot, but rather powerfully reveals the regions that have been over-explored, where the likelihood of making a new discovery or invention is vanishingly low. In this way, our characterization of the high-dimensional space of discoveries and inventions, combined with the validation of surprise as a core principle of unfolding scientific and technology growth, reveals the possibility of negative crowdsourcing, where researchers can exploit the crowd estimate of prior fruitfulness to identify where not to look for important opportunities.

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