Accelerating Scientific Data Exploration via Visual Query Systems

Doris Jung-Lin Lee, John Lee, Tarique Siddiqui, Jaewoo Kim, Karrie Karahalios, Aditya Parameswaran
Department of Computer Science
University of Illinois, Urbana-Champaign
jlee782, lee98, tsiddiq2, jkim475, kkarhal, adityagp@illinois.edu

ABSTRACT
The increasing availability of rich and complex data in a variety of scientific domains poses a pressing need for tools to enable scientists to rapidly make sense of and gather insights from data. One proposed solution is to design visual query systems (VQSs) that allow scientists to search for desired patterns in their datasets. While many existing VQSs promise to accelerate exploratory data analysis by facilitating this search, they are unfortunately not widely used in practice. Through a year-long collaboration with scientists in three distinct domains—astronomy, genetics, and material science—we study the impact of various features within VQSs that can aid rapid visual data analysis, and how VQSs fit into a scientists’ analysis workflow. Our findings offer design guidelines for improving the usability and adoption of next-generation VQSs, paving the way for VQSs to be applied to a variety of scientific domains.

INTRODUCTION
From high-throughput genome sequencing, to multi-resolution astronomical imaging telescopes, to at-scale physical testing of battery candidates, many fields of science and engineering are facing an increasing availability of large volumes of complex data [6, 10], holding the key to some of the most pressing unanswered scientific questions of our time, such as: How does a treatment affect the expression of a gene in a breast cancer cell-line? Which battery components have sustainable levels of energy-efficiency and are safe and cheap to manufacture in production? While data analysis is central to a scientist’s knowledge discovery process, scientists often lack the extensive experience to deal with data of this scale and complexity in a way that can facilitate rapid insight discovery [25].

To explore their data, many scientists currently create visualizations, either programmatically using tools (such as ggplot or matplotlib), or direct manipulation interfaces (such as Excel or Tableau) [11, 31, 41]. In either case, scientists are required to specify exactly what they want to visualize. For example, when trying to find celestial objects corresponding to supernovae, which have a specific pattern of brightness over time, scientists need to individually visualize the brightness of each object (often numbering in the thousands) until they find ones that match. Similarly, when trying to infer relationships between two physical properties for different subsets of battery electrolytes, scientists need to individually visualize these properties for each subset (out of an unbounded number of such subsets) until they identify relationships that make sense to them. This process of manually exploring a large number of visualizations is especially overwhelming for scientists who do not have extensive knowledge about their dataset.

One potential solution for this challenge of manually exploring a large collection of visualizations is systems that allow users to specify desired visual patterns, via a high-level specification language or interface, with the system automatically traversing all potential visualization candidates to find and return those that match the specification. We define such systems to be Visual Query Systems, or VQSs for short. There are a number of VQSs that have been introduced in the literature [20, 21, 30, 42, 46, 52]. One such VQS developed by us is zensage [46], which supports multiple modes of specification, including a sketching canvas where users can draw a pattern of interest, or drag and drop an existing visualization onto the same canvas, with the system finding visualizations that are similar to the queried pattern. Similarly, Google Correlate [30] and QuerySketch [52] allow users to draw a trend of interest, with the system automating the search to find matching visualizations.

Overall, VQSs appear to be an ideal fit for the challenge of visualization exploration described earlier—in that it automates the painful manual exploration of visualizations to find desired patterns. However, to the best of our knowledge, VQSs are not very commonly used in practice. Our paper seeks to bridge this gap between current research on VQSs and how they can actually be used in practice, as a first step towards the broad adoption of VQSs in data analysis. In this paper, we present findings from a series of interviews, cognitive walkthroughs, participatory design, and user studies with scientists from three different scientific domains—astronomy, genetics, and material science—through a year-long collaboration. These scientific use cases present a diverse set of goals and datasets that could benefit from a VQS. Our three main research questions are as follows:

RQ1: What are the challenges in existing scientific data analysis workflows that could be potentially addressed by a VQS?

Via cognitive walkthroughs and interviews, we gained an understanding of the data analysis workflows presently employed by our scientists, their needs, and the challenges they face. We
identified opportunities where a VQS could help accelerate their analysis, by helping them discover insights, gain intuition, or provoke directions for exploration. Finally, we determined the types of research questions and dataset properties that would be most suitable for exploration on VQSs.

**RQ2: What types of interface capabilities are necessary to develop VQSs into a useful component of data analysis?**

Via participatory design, we distilled a set of key features that our scientist participants would need for VQSs to be useful and usable within their data analysis workflows. Working with the scientists closely, we developed 20 additional features they proposed by building on top of our open-source VQS, Zenvisage [46, 47]. Unlike some of the other VQSs, Zenvisage is more recent, is open-source, is a general-purpose visual exploration system (unlike the other tools that only allow exploration of a fixed set of trends), and also provides more sophisticated querying modalities and high-level summaries. The features we developed address challenges shared across multiple use-cases, ranging from additional querying modalities, to features that support a more integrated workflow, to improving the interpretability of the system output, not all of which were supported by prior VQSs in the literature. We interacted with the participants on a regular basis to gather feedback on our VQS and understand how they envision themselves using it.

**RQ3: How can VQSs accelerate scientific insights and fit within the context of existing data analysis workflows?**

Our collaborative design experience culminated in a full-fledged VQS capable of provoking rapid iterations of different data operations and hypotheses that enable insight-discovery. To evaluate our final system, we conducted a user study with nine scientists (including those who had participated in the design), all of whom had a vested interest in using a VQS to address their research questions on their datasets. In a 1.5-hour user study, our scientist participants were able to gain novel scientific insights, such as finding characteristic gene expression profiles that confirmed the results of a related publication, and learning that the dip in an astronomical light curve is caused by saturated imaging equipment overlooked by the existing error-flagging pipeline. Participants also gained additional insights about their datasets, including debugging a mislabelled feature and finding out that the way data is aggregated across multiple experiments is erroneous on a collaborator’s dataset. We learned how VQSs could be contextualized within scientific data analysis workflows and discovered that VQSs can be used beyond the exploratory phase of analysis, for data verification, debugging preliminary datasets, and performing sanity-checks on downstream models.

As most existing VQSs are evaluated in a standalone fashion via artificial tasks and datasets, to the best of our knowledge, our study is the first to holistically examine how VQSs can be used in practice and integrated into existing data analysis workflows. From these experiences, we advocate common design guidelines and end-user considerations when building the next generation VQSs.

**RELATED WORK**

Our work is inspired by prior literature in VQSs and evaluation methods for visualization systems.

**Visualization and Visual Query Systems**

Visualization systems often support powerful direct-manipulation interfaces that enable users to specify their desired visual encoding and data subset for generating a visualization [3]. However, during data exploration, users might only have a high-level hypothesis that they want to address, rather than specific instances of what they want to visualize.

To address this issue, recent studies have explored the use of visualization recommendations to accelerate data exploration. The techniques used include using statistical and perceptual measures [27, 53, 54], past user history [15], and visualizations that look “different” from the rest [24, 50, 51, 55].

Another class of visualization systems enable the user to specify the desired pattern via some high-level specification language or interface, with the system returning recommendations of visualizations that match, instead of providing generic visualization recommendations—we call these VQSs. For example, sketching to specify the desired “shape” of a visualization, is one example of an intuitive specification interface, with the system returning visualizations that look similar [1, 21, 30, 42, 52]. Other work has explored the types of shape features a user may be interested in for issuing more specific queries [9, 17]. Other ways of specifying patterns include box constraints for range-queries [20], regular expressions [57], and natural language [13]. While these systems have been shown to be effective for dynamic querying in controlled lab studies, they have not been evaluated in-situ on real-world use cases. In this work, we additionally investigate how VQSs complement other common interactions in visual data analysis, and scientists’ existing workflows.

**Evaluation Methods For Visualization Systems**

Visualization systems are often evaluated using controlled studies that measure the user’s performance against an existing visualization baseline [39]. Cognitive measures such as insight time [35, 56] have been developed to capture how well users perform on a task against existing baselines. However, since the operations, hypotheses generated, and insights obtained through exploratory analysis are variable and subjective to individual users and their analytic goals, it is impossible to define tasks beforehand and compare across control groups. Techniques such as artificially inserting “insights” or setting predefined tasks for example datasets work well for objective tasks, such as debugging data errors [23, 36], but this contrived method is unsuitable for trying to learn about the types of real-world queries a user may want to pose on a VQS. In order to make the user study more realistic, we opted for a qualitative evaluation where we allowed participants to bring a dataset that they have a vested interest in to address an unanswered research question.

1These systems recommend visualizations based on the assumption that users are interested in seeing visualizations that maximally-deviates from some reference visualization.
Due to the unrealistic nature of controlled studies, many have proposed using a more multi-faceted, ethnographic approach to understand how analysts perform visual data analysis and reasoning [28, 33, 39, 45]. For example, multi-dimensional, in-depth, long-term case studies advocate the use of interviews, surveys, logging and other empirical artifacts to create a holistic understanding of how a visualization system is used in its intended environment [45]. Some papers have explored designing visualization and collaborative tools for scientific workflows through individual case studies, e.g., [7, 40]. Similarly, in our work, real-world case studies help us situate how VQSs could be used in the context of an existing analysis workflow.

We adopt participatory design practices in this work: participatory design “allows potential users to participate in the design of a system that they will ultimately use” [16, 32]. Participatory design has been successfully used in the development of interactive visualization systems in the past [5, 8]. In this work, we collaborated with scientists early on to develop features in zenvisage that address their analysis needs.

**METHODS**

We adopted a mixed methods research methodology that draws inspiration from ethnographic methods, iterative and participatory design, and controlled studies [22, 29, 32, 45] to understand how VQSs can accelerate scientific data analysis. Our methodology served to address the research questions outlined in the introduction. Working with researchers from three different scientific research groups, we (RQ1) identified the needs and challenges of scientific data analysis and the potential opportunities for VQSs to fit in, via interviews and cognitive walkthroughs. We further (RQ2) extended an existing VQS, zenvisage, with features for scientists via participatory design.

After incorporating desired features into our VQS over the period of a year, we (RQ3) conducted a qualitative evaluation to study how our improved VQS affected the way the users explore their data. It is interesting to note that not all of the features suggested by the participants were found to be useful during our evaluation.

| Subject | ID | Participatory design participant | Position | Years of experience in subject area | Familiarity with dataset (1-5) |
|---------|----|----------------------------------|----------|------------------------------------|-------------------------------|
| astro   | A1 | Yes                              | Research scientist | 10 | 3 |
|         | A2 | No                               | Postdoc   | 8 | 5 |
| genetics| A3 | No                               | Postdoc   | 8 | 5 |
|         | G1 | Yes                              | Grad student | 4 | 4 |
|         | G2 | No                               | Grad student | 2 | 2 |
|         | G3 | Yes                              | Professor  | 10 | 2 |
| matsci  | M1 | Yes                              | Postdoc   | 4 | 5 |
|         | M2 | Yes                              | Professor  | 10 | 5 |
|         | M3 | Yes                              | Grad student | 3 | 5 |

Table 1. Participant information. The Likert scale used for dataset familiarity ranges from 1 (not at all familiar) to 5 (extremely familiar).
UNDERSTANDING SCIENTIFIC DATA ANALYSIS

In this section, we address RQ1 by understanding the limitations and opportunities in existing scientific data analysis workflows in three research areas. We begin by describing the participants in these areas.

Participants, Datasets and Workflows

We recruited participants by reaching out to research groups who were interested in using VQSs for exploring their data via email. We summarize the common properties and differences of these three groups of researchers in Figure 1 and the desirable characteristics common to these datasets suitable for VQSs in the Discussion section. Six scientists from three research groups participated in the design of zemisage. The evaluation study participants included these six scientists, along with three “blank-slate” participants who had never encountered zemisage before. While participatory design subjects actively provided feedback on zemisage with their data, they only saw us demonstrating their requested features and explaining the system to them, rather than actively using the system on their own. So the evaluation study was the first time that all nine of the participants used zemisage to explore their datasets. We list the participants in Table 1, and refer to them by their anonymized ID as listed in the table. On average, the participants had more than 8 years of experience working in their respective fields.

The research questions and objectives of the participants were diverse even among those in the same subject area and using the same dataset. Examples of research questions included:

- Understanding the gene expression profiles of breast cancer cells that exhibit induced, transient, and repressed patterns after a particular treatment.
- Studying common patterns among stars that exhibit planetary transits versus stars that don’t from the Kepler space telescope.
- Identifying battery solvents with favorable properties and mass production potential through studying how changes in certain chemical properties correlate to changes in other chemical properties.

The pre-study survey with the participants showed that out of all of the steps in their data analysis workflow2, they spend the most time computing statistics and creating visualizations. The main bottlenecks cited in their existing workflow included the challenge of dealing with large amounts of data, writing custom processing and analysis scripts, and long turnaround times incurred by making modifications to an upstream operation in a segmented workflow.

During the participatory design process, we collaborated with each of the teams closely with an average of two meetings per month, where we learned about their datasets, objectives, and how VQSs could help address their research questions. A detailed timeline of our engagement with the participants and the features inspired by their use cases can be found in

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2 www.nasa.gov/mission_pages/kepler/main/index.html
3 This includes viewing and browsing data, data cleaning and wrangling, computing statistics, data visualization, and model building or machine learning.

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Figure 3. Participants provided datasets they were exploring from their domain, whereby they had a vested interest to use a VQS to address their own research questions. We describe the three scientific use cases below.

Astronomy (astro): The Dark Energy Survey (DES) is a multi-institutional project with over 400 scientists. Scientists use a multi-band telescope that takes images of 300 million galaxies over 525 nights to study dark energy [12]. The telescope also focuses on smaller patches of the sky on a weekly interval to discover astrophysical transients (objects whose brightness changes dramatically as a function of time), such as supernova explosions or quasars. The output is a time series of brightness observations associated with each object extracted from the images observed.

For over five months, we worked closely with an astronomer on the project's data management team working at a supercomputing facility. The scientific goal is to identify a smaller set of potential candidates that may be astrophysical transients in order to study their properties in more detail. These insights can help further constrain physical models regarding the formation of these objects.

Genetics (genetics): Gene expression is a common data type used in genomics and is obtained via microarray experiments. In these experiments, a grid containing thousands of DNA fragments are exposed to stimuli and measurements for the level at which a gene is expressed are recorded as a function of time. The data used in the participatory design sessions was the gene expression data over time for mouse stem cells aggregated over multiple experiments, downloaded from an online database4.

We worked with geneticists (a graduate student and a PI) at a research university over three months who were using gene expression data to better understand how genes are related to phenotypes expressed during early development [14,37]. They were interested in using zemisage to cluster gene expression data before conducting analysis with a downstream machine learning workflow.

Material Science (matsci): We collaborated with material scientists at a research university who are working to identify solvents that can improve battery performance and stability. These scientists work with large datasets containing over 25 chemical properties for more than 280K different solvents obtained from simulations. Once they have identified a solvent that also produces favorable results in an experiment, they identify other solvents with similar properties, which may be cheaper or safer to manufacture at an industrial scale.

We worked closely with two graduate students and a PI for over a year to design a sensible way of exploring their data using our VQS5. Each row of their dataset represents a unique solvent, and consists of 25 different chemical attributes. They wanted to use zemisage to identify solvents which have similar properties to known solvents but are more favorable (e.g.

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4 ncbi.nlm.nih.gov/geo/
5 Note that while we have interacted with the matsci participant during the initial development stage, the participatory design formally started in June 2016
Since astronomical datasets are often terabytes in scale, they are often processed and stored in highly specialized data management centers in supercomputing centers. The collaboration’s data management team has created a command-line interface that enables users to easily query, browse, and download their data. After the data is downloaded, most of the work is done programmatically through Python in an interactive Jupyter notebook environment. The astronomer inspects the data schema, performs data cleaning and wrangling, computes relevant statistics, and generates visualizations to search for anomalies or objects of interest, as shown in Figure 4a.

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Cognitive Walkthrough Sessions
Cognitive walkthroughs highlight the existing workflows and behavior that participants have adopted for conducting certain tasks [34]. In our case, we observed the participants as they conducted a cognitive walkthrough demonstrating every component of their current data analysis workflow.

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While an experienced astronomer who has examined many transient light curves can often distinguish an interesting transient object from noise by sight, they must visually examine and iterate through large numbers of visualizations of candidate objects. Manual searching is time-consuming and error prone as the majority of the objects will not be astronomical transients. Participant A1 was interested in zenvisage as he recognized how specific pattern queries could help scientists directly search for these rare objects.

If an object of interest or region is identified through the visual analysis, then the astronomer may be interested in inspecting the image of the region for cross-checking that the significant change in brightness of the object is not due to an imaging artifact. This could be done using a custom built web-interface that facilitates the access of cutout images for a queried region of the sky.

Genetics: Participant G1 processes the raw microarray data by using a preprocessing script written in R, where they (i) sub-select 144 genes of interest, (ii) clean up an experimental artifact due to measurements on multiple probes, (iii) log-transform the raw data to show a more distinct shape profile for clustering, (iv) normalize the gene expression values into the range of 0 to 1, and (v) perform Loess smoothing with default parameters to reduce the noise in the data. To analyze the data, the preprocessed data is loaded into a desktop application for visualizing and clustering gene expression data. G1 sets several clustering and visualization parameters on the interface before pressing a button to execute the clustering algorithm. The cluster visualizations are then displayed as overlaid time series for each cluster, as shown in the visualization in Figure 4b. G1 visually inspects that all the patterns in each cluster look “clean” and checks the number of outlier genes that do not fall into any of the clusters. If the number of outliers is high or the visualizations look unclean, they rerun the clustering by increasing the number of clusters. Once the visualized clusters look “good enough”, G1 exports the cluster patterns into a csv file to be used as features in their downstream regression tasks.

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5 [github.com/mgckind/easyaccess]
6 [jupyter.org]
7 [www.cs.cmu.edu/~jernst/stem/]

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Figure 3. Participatory design timeline for the scientific use cases. In all three of the scientific use cases, there was a period of time for establishing the minimum data and systems requirements for understanding how a visual query system can be used for the particular scientific use case. These include understanding the types of data suitable for the system, cleaning data, and denoising procedures for the chosen dataset. The minimum system requirements include features that are required for the data to be visualized appropriately. After seeing the data being displayed for the first time in our system, the scientist naturally begins to envision the types of queries that they would like to make and ways that finer query specifications and system controls that could help better address their science questions.
Prior to the study, the student (G1) and PI (G3) spent over a month attempting to determine the best number of clusters for their upstream analysis based on a series of static visualizations and statistics computed after clustering. While regenerating their results took no more than 15 minutes every time they made a change, the multi-step, segmented workflow meant that all changes had to be done offline, so that valuable meeting time was not wasted trying to regenerate results. The team had a vested interest in participating in the design of zenvisage as they saw how the interactive nature of VQSs and the ability to query other time series with clustering results could dramatically speed up their collaborative analysis process.

Material Science: Participant M1 starts his data exploration process with a list of known and proven solvents as a reference. For instance, he would search for solvents which have boiling point over 300 Kelvins and the lithium solvation energy under 10 kcal/mol using basic SQL queries. This would help him narrow down the list of solvents, and he would continue this process with other properties. The scientist also considers the availability and the cost of the solvents while exploring the dataset. When the remaining list of the solvents is sufficiently small, he drills down to more detail (e.g., such as looking at the chemical structure of the solvents to consider the feasibility of conducting experiments with the solvent). While he had identified potential solvents through manual lookup and comparison, the process lacked the ability to reveal complicated trends and patterns that might be hidden, such as how the change in one attribute can affect the behavior of other attributes of a solvent. M1 was interested in using a VQS as it was infeasible for him to manually compare between large numbers of solvents and their associated properties manually.

THEMES EMERGING FROM PARTICIPATORY DESIGN

In the previous section, we gained an understanding of the current analysis workflows employed in the three use cases. Next, to address RQ 2, we employed participatory design with our scientists to incorporate key features missing in our original VQS, and unaddressed in their current workflows. Of the 20 features we implemented, 16 were suggested by multiple use cases. We discovered three central themes encapsulating these features that are important to facilitate rapid hypothesis generation and insight discovery, but are missing in prior VQSs, described next. While some of our findings echo prior work on system-level taxonomies of visualization tasks [4, 19], we highlight how specific analytic tasks and interaction features could be used to enhance VQSs in particular. In particular, we learned that participants wanted more control over the internals of the systems and an integrated workflow that helped streamline their analysis when using VQSs.

Uninterrupted workflow

Our cognitive walkthroughs revealed that in many participants’ existing workflows, they switched between parameter specification, code execution, and visualization comparisons. The non-interactive nature of these segmented workflows has been shown to incur a large cognitive barrier during exploratory data analysis [26]. Moreover, data-cleaning emerged as a common pain-point, echoing prior work [18, 24].

Integrative preprocessing through interactive smoothing (astro, matsci)

While zenvisage does not attempt to solve all of the pre-processing issues that we faced during participatory design, we identified that data smoothing is a common data cleaning procedure [48] that would benefit from a tight integration between pre-processing and visual analysis.

To address this issue, we developed an interface for users to interactively adjust the data smoothing algorithm and parameters on-the-fly to update the resulting visualizations accordingly (Figure 5i). This was applied to the matsci and astro use cases, as both had noisy and dense observational data.

Facilitating export for downstream analysis (astro, genetics)

Since zenvisage is designed to be an exploratory tool that suggests potential directions (rather than a one-shot analysis), we asked participants how they envisioned themselves using zenvisage in their workflow. Both the astro and genetics participants wanted to use VQSs as a way to identify interesting objects or characteristic patterns, which they will later feed into a more advanced downstream pipeline.

To smoothen the transition between the VQS and their downstream analysis, we implemented export functionalities for downloading the similarity, representative trend and outlier results as csv files (Figure 5m). Individual visualizations can also be downloaded as figures to facilitate easier sharing of visualization results with collaborators (Figure 5d).

Sophisticated data operations in a VQS

The initial VQS did not satisfy the participants’ needs for sophisticated data operations. They wanted more ways to explore their data, either through additional querying methods, or the ability to query on a subset of data.

Increasing the expressiveness of querying capabilities (all)

While the interactions in our original system enables simple queries, many scientists were interested in extending their querying capabilities, either through different modalities of querying or through more flexible query expression.

Input Equations: Our matsci participants expressed that some solvents can have analytical models that characterize the relationships between chemical properties. They wanted to find solvents that satisfied these relationships. We implemented a feature that plots a given function (e.g. $y = x^2$) on the canvas, which is then used as input for similarity search (Figure 5n).

Upload Pattern as Query: While the input equation is useful when simple analytical models exist, this may not be true for other domains. In these cases, users can upload a query pattern of a sequence of points (Figure 5a). This is useful for patterns generated from advanced computational models used for understanding scientific processes, usually as part of the downstream analysis of the exploratory workflow.

Consider/Ignore x-range: We improved query specification by allowing users to change how the shape-matching criterion is applied. For finding supernovae, A1 primarily cared about the existence of a peak above a certain amplitude with an appropriate width of the curve, rather than the exact time that the event occurred, leading them to use the consider x-range
Figure 5. Our VQS after participatory design, which includes: querying functionalities via (a) patterns and (n) equations; query specification mechanisms including (b) Dynamic class creation, (j) Filtering, and (e) x-range invariance, selection and filtering; the ability to preprocess via (i) interactive smoothing; visualization display options (c); system parameter options (g, i, f); and the ability to export data outputs. Prior to the participatory design, zenvisage only included a single sketch input with no additional options. zenvisage also displayed representative patterns and outlier patterns.

Figure 6. An example of four created dynamic classes. (a) shows four different classes with different Lithium solvation energies and boiling point attributes based on user-defined custom ranges. (b) the user can then hover over the visualizations to see the attribute ranges for each visualization. The visualizations of dynamic classes aggregate across all the visualizations that lie in that class.
Finer System-level Control and Understanding

During the participatory design exercise, we found that many of the features suggested by the participants indicated they wanted finer control of the system. Prior work in direct manipulation visual interfaces has suggested that finer-grained control enabled users to discover patterns and rapidly generate hypothesis based on visual feedback [43, 44].

Controlling what the VQS does internally (all)

In addition to query and dataset specifications, users also wanted the ability to modify the model parameters in zenvisage. Our findings echoed Chuang et al. [8], which showed that the ability to modify the model can facilitate interpretation and trust in model-driven visualizations, especially during early-stage exploration. These model parameter options include the ability to change the choice of similarity metrics (Figure 5f), the cluster size in the representative patterns (Figure 5g), setting a minimum similarity threshold for displaying the search results (Figure 5h), and the ability to tune the smoothing algorithm and parameter (Figure 5i).

Displaying interpretable outputs explaining how VQS arrived at recommended visualizations (all)

Explanatory system outputs include displaying similarity scores of the outputs, the number of datapoints in each cluster, and overlaying the original query sketch on the return visualization for comparison. We further provided display-related options for plotting modifications, including displaying error bars, and toggling between a scatterplot and line chart view.

FINAL EVALUATION STUDY: METHODOLOGY

Our final evaluation study addresses RQ3—whether our new and improved VQS helps accelerate insight, and how it could fit into real analysis workflows. Participants for the evaluation study were recruited from each of the three aforementioned research groups. Prior to the study, we asked the potential participants to fill out a pre-study survey to determine their eligibility. Eligibility criteria included: being an active researcher in the subject area with more than one year of research experience, and having worked on a research project involving data of the same nature as that used in the participatory design. Four of the user studies were conducted remotely.

Participants had the option of exploring their own dataset or an existing dataset that they provided to us during the participatory design process. All four blank-slate participants opted to explore their own datasets. After loading their dataset, we emailed them a screenshot of a visualization from our tool to verify that we configured the system to meet their needs.

At the start, participants were provided with an interactive walk-through explaining the details of the features offered in our VQS. The participants were then given approximately ten minutes to experience a guided exploration of our VQS with a preloaded real-estate example dataset from Zillow [2]. This dataset contained housing data for various cities, metropolitan areas, and states in the U.S. from 2004-15. After familiarizing themselves with the tool, we loaded the participant’s dataset and suggested an appropriate choice of axis to begin the exploration. Participants were encouraged to talk-aloud during the data exploration phase.

During the exploration phase, participants were informed that they could use other tools as needed. If the participant was out of ideas, we suggested one of the ten main operations that they had not yet covered. If any of these operations were not applicable to their specific dataset, they were allowed to skip the operation after having considered how it may or may not be applicable to their workflow. The user study ended after they covered all ten main functionalities. On average, the main exploration phase lasted for 63 minutes. After the study, we asked them open-ended questions about their experience.

Data Collection & Analysis

We recorded audio, video screen captures, and click-stream logs of the participant’s actions during the evaluation study. We analyzed the transcriptions of these recordings through a thematic coding process by two of the authors.

- Insight (Science) [IS]: Insight that connected back to the science (e.g. “This cluster resembles a repressed gene.”)
- Insight (Data) [ID]: Data-related insights (e.g. “A bug in my data cleaning code generated this peak artifact.”)
- Provoke (Science) [PS]: Interactions or observations made using zenvisage that provoked a scientific hypothesis to be generated.
- Provoke (Data) [PD]: Interactions or observations made using zenvisage that provoked further data actions to continue the investigation.
- Confusion [C]: Participants were confused during this part of the analysis.
- Want [W]: Additional features that participant wants, which is not currently available on the system.
- External Tools [E]: The use of external tools outside of zenvisage to complement the analysis process.

In addition, for each of the ten features in the user study, we categorized them into one of the four usage types:

- Practical usage [P]: Features used in a sensible and meaningful way during user study.
- Envisioned usage [E]: Features which could be used practically if the envisioned data was available or if they conducted downstream analysis, but was not performed due to limited time during the user study.
- No usage [N]: Features that do not make sense for the participant’s research question or dataset.

The results based on this thematic coding is depicted in Figure 7 and 8, and will be discussed in the next section.

FINAL EVALUATION STUDY: RESULTS AND DISCUSSION

We now describe our study results for RQ3. To contextualize our study results with respect to prior work on how analysts make sense of data, we employ Pirolli and Card’s [38] information foraging framework for domain-experts. Pirolli and Card’s notional model distinguishes between information processing tasks that are top-down (from theory to data) and bottom-up (from data to theory). They further characterize the trade-offs between three central activities in the information processing framework: searching, exploring, and evaluating.
foraging process: exploring, enriching, and exploiting. Exploring is a bottom-up process that involves gathering more information during the analysis. In the context of zenvisage, exploring includes viewing representatives and outliers, incidental viewing of other visualizations, and querying via drag-and-drop and pattern-loading. Enriching is a top-down process involving tasks that narrow down the space of analysis, such as filtering, dynamic class creation, query specification, and querying via input equations and sketching. Exploiting involves spending time inspecting the results in more detail, including interpreting each visualization in greater detail or making plotting changes that offer another perspective (smoothing, display, and interpretability settings).

Our study results fall into two main themes. First, we discuss how VQS features were used in practice to achieve scientific insights. We find that VQSs can enable rapid, fluid iteration, catalyzing new questions or insights; that different querying modalities in VQSs supported different forms of exploration; and that expressive querying allowed participants to compose novel analysis patterns. Second, we determine where VQSs fit into real data analysis workflows. We find that VQSs can be used for a range of tasks that go beyond just exploration; that participants used the outputs from VQSs in various ways; and that VQSs are most appropriate for certain types of datasets.

**Actionable VQS features for scientific insight**

The ability to rapidly experiment with large numbers of hypotheses in real time is a crucial step in the agile creative process in helping analysts discover actionable insights [44]. Five out of nine participants discussed how the dynamic, interactive update of the visualization in zenvisage was the main advantage for using VQSs over their original workflow.

Integrated workflow results in more experimentation.

Our participants’ original workflow often requires them to compare between many visualizations manually through separate analysis and visualization steps. Three of the participants cited that this artificial segmentation was one of their chief bottlenecks. The cognitive overhead from the segmented workflow made them more hesitant to visualize the results of different parameters and data operations, as A2 noted:

The quick visualization is something that I could not do on my current framework. I could not query as fast as you do; I need to wait for it, plot, and then compare. Every time I plot, I need to define subplots for 12 visualizations, then its slower. That’s the reason why I sometimes plot less, and I rely more on the statistics from the likelihood tests. Sometimes I plot less than I really should be doing.

In Figure 7, we also see that our VQS provoked users to generate many data operations (PD) and hypotheses (PS).

**Rapid insights via VQSs catalyze new questions, hypotheses, and actions.**

A common theme that we found across the genetics participants is that they often gain their intuition about the data from the representative trends. They first identified that the three representative patterns shown in zenvisage—induced genes (profiles with expression levels staying up), repressed genes (started high but went down), and transients (go up and then come down at different time points)—corresponded to the same three groups of genes discussed in a recent publication.

The clusters provoked G2 to generate a hypothesis regarding the properties of transients: “Is that because all the transient groups get clustered together, can I get sharp patterns that rise and ebb at different time points?” To verify this hypothesis, G2 increased the parameter controlling the number of clusters and noticed that the cluster no longer exhibited the clean intuitive patterns he had seen earlier. G3 expressed a similar sentiment and attempted to identify different clusters. She proceeded by inspecting the visualizations in the cluster via drag-and-drop and found a group of genes that all transitioned at the same timestep, while others transitioned at different timesteps. G3 described the process of using VQSs as doing “deceptive work” that provoked her to generate further scientific hypotheses as well as data actions.

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**Bottom-up vs. top-down querying**

Our interactions with the scientists showed that different modalities for inputting a query can be useful for different problem contexts. Overall, bottom-up querying via drag-and-drop was more intuitive and commonly used than top-down querying via sketching or input equations. For instance, only two out of our nine users found a practical use for query by sketching. The main reason why participants did not find sketching useful was because they often do not start off their analysis with a pattern in mind. Later, their intuition about what to query is derived from other visualizations that they see in the VQS, in which case it made more sense to query using those visualizations as examples directly (via drag-and-drop). In addition, even if a user has a query pattern in mind, sketch queries can be ambiguous [9] and hard to draw (e.g., A2 looked for a highly-varying signal enveloped by a sinusoidal pattern indicating planetary rotation). We suspect that this is the reason why existing sketch-to-query systems are not used commonly in practice, despite extensive research.

Despite functional fitting being common in scientific data analysis, Figure 8 shows that querying by equation is also unpopular for the same reason as a sketched query. In addition, the visualizations for both astro and genetics exhibit complex processes that could not be written down analytically. However, even when analytical relationships do exist (in the case of matsci), it is challenging to formulate functional forms in an ad-hoc manner.

On the other hand, many participants envisioned use cases for pattern loading, including comparing visualizations between different experiments, species, or surveys, querying with known patterns from an external reference catalog (e.g., important genes of interest, objects labelled as supernovae), specifying a more precise query that captures the exact shape features (e.g., amplitude, width of peak) which can not be precisely drawn as a sketched pattern, and verifying the results of a simulation or downstream analysis by finding similar patterns in the existing dataset. Similarly, drag-and-drop was the querying mechanism used most frequently by the participants. Examples of practical uses of drag-and-drop includes inspecting the top-most similar visualizations that lie in a cluster and finding visualizations that are similar to an object of interest that exhibits the desired pattern.

While the usage of each querying feature may vary from one participant to the next, generally, drag-and-drop and pattern upload are considered bottom-up approaches that go from data to theory by enabling users to query via examples of known visualizations. For top-down approaches such as query by sketching and input equations, the user starts with an theoretical intuition about how their desired patterns should look like, then conducts a search based on that. Our results indicate that bottom-up querying approaches are preferred over top-down when the users have no desired patterns in mind, which is commonly the case for exploratory data analysis.

**Top-down and bottom-up faceted exploration**

All participants either envisioned a use case or utilized filtering or dynamic class creation to explore and compare subsets of their data. A1 expressed that even though the filtering step could be easily done programmatically on the dataset and reloaded into zenvisage, the filter constraint was a powerful way to dynamically test their hypothesis. Interactive filtering lowers the barrier between the iterative hypothesis-then-compare cycle, thereby enabling participants to test conditions and tune values that they would not have otherwise modified as much. During the study, participants used filtering to address questions such as: “Are there more genes similar to a known activator when we subselect only the differentially expressed genes (e.g., DIFFEXP=1)” (G2) or “Can I find more supernovae candidates if I query only on objects that are bright and classified as a star (e.g., flux>10 AND CLASS_STAR=1)” (A1). Three participants had also used filtering as a way to pick out individual objects of interest to query with. For example, G2 set the filter as gene=’9687’ and explained:

> We know that this gene is regulated by the estrogen receptor, when we search for other genes that resembles this gene, we can find other genes that are potentially affected by the same factors.

As shown in Figures 7 and 8, participants with the top-most provoked data actions (A1,A3,G2) made heavy use of filtering to explore different subsets of the data.

While filtering enabled users to narrow down to a selected data subset, dynamic class creation enabled users to compare the relationships between multiple physical attributes and between subgroups of data. For example, M2 divided the solvents in the database to eight different classes based on the voltage properties, state of matter at room temperature, and viscosity levels, by dynamically setting the cutoff values to create these classes. By exploring the created custom classes, M2 learned that the relationship between viscosity and lithium solvation energy is independent of whether a solvent belongs to the class of high voltage or low voltage solvents. M2 cited that dynamic class creation was central to learning about this previously-unknown property of these two attributes:

> All this is really possible because of dynamic class creation, so this allows you to bucket your intuition and put that together. […] I can now bucket things as high voltage stable, liquid stable, viscous, or not viscous and start doing this classification quickly and start to explore trends. […] And look how quickly we can do it! Quite good!

Participants employed a mix of bottom-up and top-down approaches when facetting through data in VQS, including narrowing the search space based on some intuition about a phenomena, selecting individual visualizations, or specifying high-level groupings to compare and query with.

**The need to perform comparisons across multiple collections of visualizations on different data attributes.**

All participants wanted the ability to perform comparisons across multiple collections of visualizations on different data attributes, including comparison tasks such as: comparing between genes that belong to different functional groups (G1,G3); comparing between stars that harbor planets (which exhibits a transit pattern) and stars that don’t (A2); comparing similarity and dissimilarity between two different sets of y measurements, such as time series of gene expression v.s. hypersensitivity (G2), stellar fluxes across different bands (A1); and comparing the correlation between different chemical properties for different solvent groups (M2).
These complex tasks are akin to the queries in the Zenvisage Query Language (ZQL) [47], which we did not demonstrate to our participants in our VQS to avoid confusion. To complete these tasks using our VQS, participants would have had to use the querying interface multiple times while also remembering past results, which can be error-prone. Developing sensible interactions to map user intentions to sophisticated query languages like ZQL is an important direction for future work.

**Novel workflows focusing on one central foraging act.**

In addition to observations regarding how participants use features within our VQS, we also find that participants often create unexpected workflows that chain together multiple interactions, controls, and queries in order to address a higher-level research question. These behaviors can be explained in terms of the foraging acts (exploring, exploiting, and enriching) introduced by Pirolli and Card [38]. We find that participants often construct a central workflow, then they continue to perform the same workflow over and over with additional variations. Their central workflow often resembles one of the three foraging acts that aligns with the type of research question and dataset they are interested in. The variations are based on intermixing their central workflow with the other two foraging activities.

For example, the geneticists were mostly interested in exploring clusters to gain an overall sense what profiles exist in the dataset and therefore queried mainly through drag-and-drop. The variations to their main workflow include changing cluster sizes and display settings to offer them different perspectives on the dataset (exploit) and filtering on data attributes (enriching). The main workflow for the astronomers in our user study involves enriching, either through the creation of groups or via filtering data subsets. The main workflow for the materials scientists involves exploiting, since they spend the majority of their efforts performing “close-reading” of individual visualizations to understand the relationships between physical variables.

**Using VQSs within a scientific data analysis workflow**

We also gained insights into how VQSs can potentially integrate with scientists’ existing workflows. We start by identifying properties of ideal datasets for VQSs.

**Large, two-dimensional, and ordinal datasets are well suited for VQSs.**

In selecting our three user groups, we spoke to participants from 12 different potential application domains ranging from connectomics to protein networks. We focused on the astro, genetics, matsci groups in this paper since their data can be viewed in a line chart format and their tasks required comparisons across many visualizations. There were many interesting potential scientific use cases that did not satisfy these criteria. For example, time-varying 2D maps representing the interactions between brain regions and protein-protein interactions are non-ordinal heatmaps, with no simple sketching analogy.

Even when the data is time series-based, some potential application domains had data characteristics that made it difficult to use a VQS. For example, a neuroscientist noted that their time series only consists of 3-5 observations, since each observation required the dissection of a mouse brain. Sparse datapoints can be difficult for existing shape matching algorithms.

**VQSs can be used beyond the exploration stage of analysis.**

Two of the five datasets used in the user study were preliminary in the sense that the scientists had performed only basic data cleaning and had not explored this dataset in great detail themselves. This enabled us to get a sense of how VQSs can be used in practice at different stages of the analysis workflow. We originally envisioned zenvisage as a tool for finding interesting patterns following which scientists could proceed to a more detailed and rigorous analysis based on these newly-obtained insights. We realized after the evaluation study that users were interested in using VQSs for more than one-step pattern-finding. This enabled us to get a sense of how VQSs can be used in practice at different stages of the analysis workflow. For example, A2 commented:

> [The VQS] fits in after the cleaning and after correcting for systematics, I will use the VQS for a first visualization, not taking the advantage of all the features that the VQS has, and then will perform a first analysis and then come back to the VQS (in this analysis I will calculate the rotational period and some other values that could help me separate out the categories in the VQS), then after I learn about the categories. In the end, I will again use the VQS to visually inspect the data.

Participants also explained where they saw VQS fit into their workflow, including (i) visualizing raw data before cleaning to learn about what types of outliers, representative trends, and artifacts are present in the data (A1,A2,G2,M3); (ii) data verification after cleaning to see if known patterns show up as expected (G1); and (iii) verifying the correctness of a simulation, by visualizing data from a simulation that is based on insights obtained using the VQS (G1,G3).

**VQSs can be used for verifying data fidelity and debugging.**

Participants often used zenvisage to verify the fidelity of their data and perform debugging. For example, G2 crosschecked that there were no data artifacts of “genes with two peaks” via sketching. Via the visualizations displayed in the result, representative, and outlier panels in zenvisage, participants were able to gain a peripheral overview of the data and spot anomalies during exploration. For example, A1 spotted time series that were too faint to look like stars after applying a filter constraint of CLASS_STAR=1. After a series of visualizations of other query results and consultation with an external database, he concluded that the dataset had been incorrectly labelled with all the stars with CLASS_STAR=0 as 1 during data cleaning.

Explanatory display outputs work closely in conjunction with finer control mechanisms so that users receive feedback on their data actions and immediately update their mental models. For example, the genetics participants modified the clustering parameters and verified that the size of each cluster still remained relatively even, in order to determine the best values of the parameters. This served as a verification mechanism that helped users build trust in the model outputs by cross checking with their intuition on what should happen to the result as they perform an operation [8]. Moreover, the dynamic, real-time update of VQSs aid rapid hypothesis generation and encourage scientists to try things that they would not have done otherwise, especially for exploratory tasks that had a low
probability of producing interesting results, such as browsing for anomalies or data verification.

**VQSs are used in conjunction with external tools.**

During the user study, four of the scientists consulted external tools outside of the VQS as a reference. Two out of the four used the external tools to compute statistics, browse related datasets, or examine other data attributes. This shows that generic VQSs are not a one-size-fits-all solution [49], and domain-specific tools are often useful to provide context.

For example, A1 saw a strange dip in the time series in the VQS and wanted to see whether it was an artifact. He first checked the database to see if there is an error flag associated with the observation of this object and learned that this object is labelled as a galaxy. Upon comparing with the other visualization in the panel in the VQS, he noticed the difference in y values and hypothesized that object was so faint that it was below the detection limit of the instrument. After going to an external software to inspect the images, he verified his hypothesis as the image was so noisy and a bright nearby star may have saturated the imaging equipment and resulting in the dip in the observations.

We identified two main reasons why scientists go to external tools to support their analysis in VQS. (1) Scientists often require multiple sources of data to test the validity of their hypothesis. For example, to determine whether a particular gene belongs to a regulatory network, G2 not only looks at the expression data in the VQS but also enrichment testing and knockout data. Visualizing these data often requires specialized tools and isn’t supported by a generic VQS. To enable smoother transitions between tools, several participants expressed that VQSs should bookmark and track the history of visualizations that they had found interesting. (2) Scientists also use many different data attributes to better understand the data that they are visualizing in the VQS and further develop their hypotheses. Four participants wanted the VQS to support data summaries (histograms, statistics) on the non-visualized attributes to assist them with choosing appropriate values for filtering data subsets and class creation. For instance, A2 used his Jupyter Notebook during exploration to obtain summary statistics on radius of a star.

*Insights derived as preliminary, and can be subjected to more robust testing or downstream modeling.*

We ask participants the types of additional analysis they plan to run downstream after obtaining insights from our VQS. Eight out of nine participants envisioned that exporting functionalities in *zenvisage* are useful for directing them to the next step of their analysis workflow. For astronomers, the post-analysis tasks involve cross-checking and inspecting individual objects of interest more closely, including using external data types such as images. A1 discussed how he plans to perform a more rigorous “blind analysis”, which involves taking the visualized data without any IDs or associated data attribute, and seeing if other statistical techniques yields the same set of interesting objects as the ones discovered visually through VQS. All genetics participants expressed that they will export the clusters and directly move onto the next stage of the analysis without additional verification, since they regard the results from VQS “simply as guidelines” (G3) that provide them with the intuition about what types of patterns exist in their dataset, before they start building advanced models. Figure 7 shows that no *matsci* participant wanted to export their data because they were more interested in insights gained from understanding relationships between chemical properties rather than finding particular solvents. The question of how analysts understand and trust the outputs of VQS depending on the objectives of their analysis is an interesting direction for future work.

**CONCLUSION AND FUTURE WORK**

In the face of a data deluge in science, many scientists struggle to leverage these large datasets to derive scientific insights. While VQSs hold tremendous promise in accelerating data exploration, they are rarely used in practice. In this paper, we worked closely with three groups of scientists to learn about the challenges they face when working with data. We extended our VQS *zenvisage* to the point where it could be effectively used for scientific data analysis.

From cognitive walkthroughs and interviews, we learned about the challenges faced in scientific data analysis, including the lack of experimentation due to segmented workflows, and having to compare between large collections of visualizations (RQ1). Through participatory design, we identified three classes of missing interface capabilities essential for employing VQSs for facilitating insight in real scientific applications, spanning expressive querying and dynamic faceting, as well as fine-grained control and understanding, along with the ability to compose flexible workflows in an integrated manner (RQ2). Finally, our evaluation study demonstrated how these features helped accelerate scientific insights, as well as how they fit in the context of data analysis workflows (RQ3). One such finding is that bottom-up querying (e.g., drag-and-drop) is preferred over top-down (e.g., sketching) for exploratory data analysis, contrary to what is commonly supported in existing VQSs. Scientists were able to use *zenvisage* for debugging errors in their data, for discovering desired patterns and trends, and for obtaining scientific insights to address unanswered research questions. By extending and evaluating VQSs to support real data analysis workflows across multiple scientific domains, we believe this work can serve as a roadmap for broad adoption of VQSs in data analysis.

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