

Accelerating Scientific Data Exploration via Visual Query System

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 interactively search for desired patterns in their datasets. While many existing VQSs promise to accelerate exploratory data analysis by facilitating this search, they are 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 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.

KEYWORDS

Visual analytics, visualization, exploratory data analysis, visual query, scientific data.

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1 INTRODUCTION

2 RELATED WORKS

3 METHODS

Motivation

We adopted a mixed methods research methodology that draws inspiration from ethnographic methods, iterative and participatory design, and controlled studies [15, 16, 23] to understand how VQSs can be used for scientific data analysis. Working with researchers from three different scientific research groups, we identified the needs and challenges of scientific data analysis and the potential opportunities for VQSs, via interviews and cognitive walkthroughs.

Visualization systems are often evaluated using controlled studies that measure the user’s performance against an existing visualization baseline [21]. Techniques such as artificially inserting “insights” or setting predefined tasks for example datasets work well for objective tasks, such as debugging data errors [10, 19], but these contrived methods are unsuitable for trying to learn about the types of real-world queries users may want to pose on VQSs. 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 [13, 14, 17, 21, 23]. In order to make the user study more realistic, we opted for a qualitative evaluation where we allowed participants to bring datasets that they have vested interests in to address unanswered research questions. Participatory design has been successfully used in the development of interactive visualization systems in the past [3, 5]. Sedlmair et al. [14] advocate that design study methodology is suitable for use cases in which the data is available for prototyping, but the task is only partially known and the information is partially in the user’s head. In that regard, our scientific use cases with VQS is well-suited for a design study methodology, as we learn about the scientist’s data and analysis requirements and design interactions that helps users translate their “in-the-head” specifications into actionable visual queries.

Participatory Design

We recruited participants by reaching out to research groups via email and word of mouth, who have experienced challenges in dealing with large amounts of data. We initially spoke to analysts from 12 different potential application areas and narrowed down to three use cases in astronomy, genetics, and material science for our participatory design study. Six scientists from three research groups participated in the design of *zenvisage*. On average, the participants had more than 8 years of research experience working in their respective fields. We list the participants in Table ??, and will refer to them by their anonymized ID as listed in the table throughout the paper.

Our initial inspiration for building a VQS came from informal discussions with academic and industry analysts. Their current workflows required analysts to manually examine large numbers of visualizations to derive insights from their data. Given these early conversations with the participants, we built a basic VQS to serve as the functional prototype in the

design study. As shown in Figure 1, this early version of *zenvisage* allowed users to sketch a pattern or drag-and-drop an existing visualization as a query, then the system would return visualizations that had the closest Euclidean distance from the queried pattern. The details of the system is described in our previous work [24, 25], which focused on the systems and scalability aspects of the VQSs.

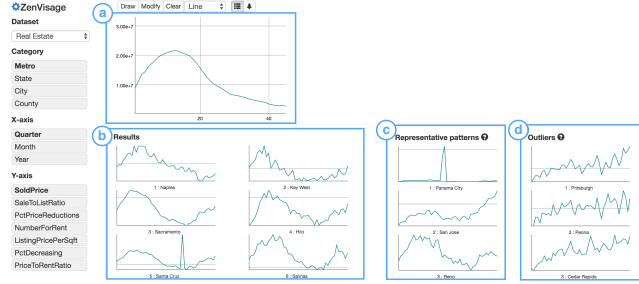


Figure 1: The *zenvisage* prototype allowed users to sketch a pattern in (a), which would then return (b) results that had the closest Euclidean distance from the sketched pattern. The system also displays (c) representative patterns obtained through K-Means clustering and (d) outlier patterns to help the users gain an overview of the dataset.

The use of functional prototypes is common in participatory design to provide a starting point for the participants. For example, Ciolfi et al.[6] studied two different alternatives to co-design (starting with open brief versus functional prototype) in the development of museum guidance systems and found that while both approaches were equally fruitful, functional prototypes can make addressing a specific challenge more immediate and focused. Our motivation for providing a functional prototype at the beginning of the participatory design sessions is to showcase capabilities of VQSs. Especially since VQSs are not common in the existing workflows of these scientists, participants may not be able to imagine their use cases without a starting point.

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 Figure 2. Participants provided datasets they were exploring from their domain, whereby they had a vested interest in using a VQS to address their own research questions. Through this process, we identified and incorporated more than 20 desired features into the VQS prototype over the period of a year.

Evaluation Study

Finally, we conducted a realistic, qualitative evaluation to study how analysts interact with different VQS components in practice. The evaluation study participants included the six scientists from the participatory design study, along with three additional “blank-slate” participants who had never encountered *zenvisage* before. While participatory design subjects actively provided feedback on *zenvisage* 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 *zenvisage* to explore their datasets.

Participants for the evaluation study were recruited from each of the three aforementioned research groups, as well as domain-specific mailing lists. 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 three 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 [1]. 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 functionalities in *zenvisage* 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.

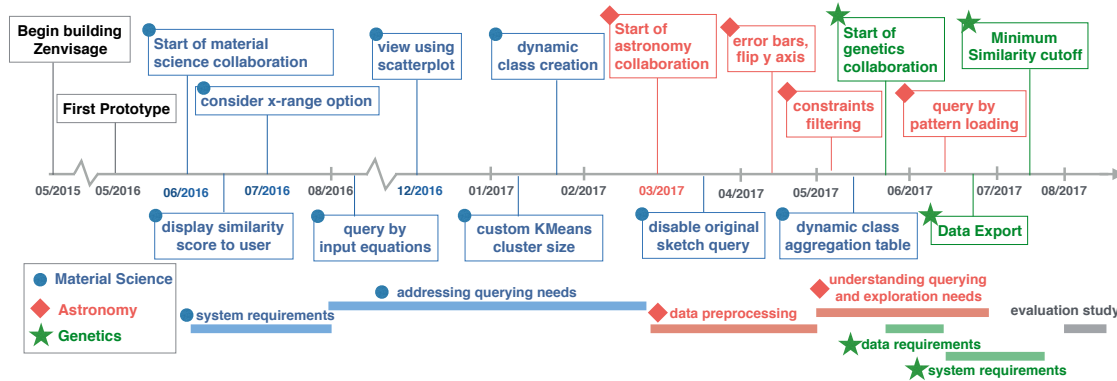


Figure 2: Participatory design timeline for the scientific use cases.

4 PARTICIPANTS AND DATASETS

During the design study, we observed the participants as they conducted a cognitive walkthrough demonstrating every component of their current data analysis workflow. In this section, we describe our study participants and their use cases to highlight the existing workflow and behavior that participants have adopted for conducting certain analysis tasks [18].

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[7]. 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 super-computing 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.

Participant A1 was interested in *zenvisage* as he recognized how specific pattern queries could help scientists directly search for these rare objects. 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 large majority of the objects are not astronomical transients.

Genetics (*genetics*)

Gene expression is a common data type used in genomics and is obtained via microarray experiments. The data used in the participatory design sessions was the gene expression

data over time for mouse stem cells aggregated over multiple experiments.. We worked with 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 [8, 20]. They were interested in using *zenvisage* to cluster gene expression data before conducting analysis with a downstream machine learning workflow.

To analyze the data, participant G1 loads the preprocessed data into a desktop application for visualizing and clustering gene expression data¹. Participant 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 ??b. G1 visually inspects that all the patterns in each cluster looks “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, she reruns the analysis by increasing the number of clusters. When 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.

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.

¹www.cs.cmu.edu/~jernst/stem/

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 280,000 different solvents obtained from simulations.

We worked closely with a graduate student, a postdoctoral researcher, and a PI for over a year to design a sensible way of exploring their data using VQSs. Each row of their dataset represents a unique solvent, and consists of 25 different chemical attributes. They wanted to use *zenvisage* to identify solvents that not only have similar properties to known solvents but also are more favorable (e.g. cheaper or safer to manufacture), as well as to understand how changes in certain chemical attributes affects them.

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 above 10 kcal/mol using basic SQL queries. This helps him narrow down the list of solvents, and move on to the other properties for similar processing. 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 could identify 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.

These observations inform our — search-browse paradigm

5 STUDY FINDINGS

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 RQ2, we employed participatory design with our scientists to incorporate key features missing in our original VQS, and unaddressed in their current workflows. 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. While some of our findings echo prior work on system-level taxonomies of visualization tasks [2, 9], we highlight how specific analytic tasks and interaction features could be used to enhance VQSs in particular.

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 [12]. In addition, since scientific research often takes place in a collaborative setting, this means that the data sense-making process could be delayed by weeks because the analysis-to-results phases needed to be rerun offline based on changes that were suggested during a meeting. Moreover, data-cleaning emerged as a common pain-point, echoing prior work [10, 11].

Integrative preprocessing through interactive smoothing:

While *zenvisage* does not attempt to solve all of the preprocessing issues that we faced during participatory design, we identified data smoothing as a common data cleaning procedure that could benefit from a tight integration between pre-processing and visual analysis. Data smoothing is a denoising procedure that generates a smoothed pattern approximating key features of the visualized trend with less noise. Smoothing also raises an interesting trade-off between the smoothness of the curve and the quality of shape-matching for VQSs. If the visualization is over-smoothed, then shape matching would return results that only loosely resemble the query pattern. However, if no smoothing is applied, then the noise may dominate the overall trend, which could also lead to bad pattern matches. In addition, it is often hard to tell what the appropriate smoothing parameter should be applied simply by visualizing a small number of sampled visualization, as one would do in an offline 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 5a). This was applied to the *matsci* and *astro* use cases, as both had noisy and dense observational data.

Facilitating export for downstream analysis: Since VQSs are designed to be exploratory tools that suggest potential directions for further analysis, rather than for performing one-shot operations, we asked participants how they envisioned themselves using VQSs 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 5b). Individual visualizations can also be downloaded by double-clicking individual figures (Figure 5c) to facilitate easier sharing of visualization results with collaborators.

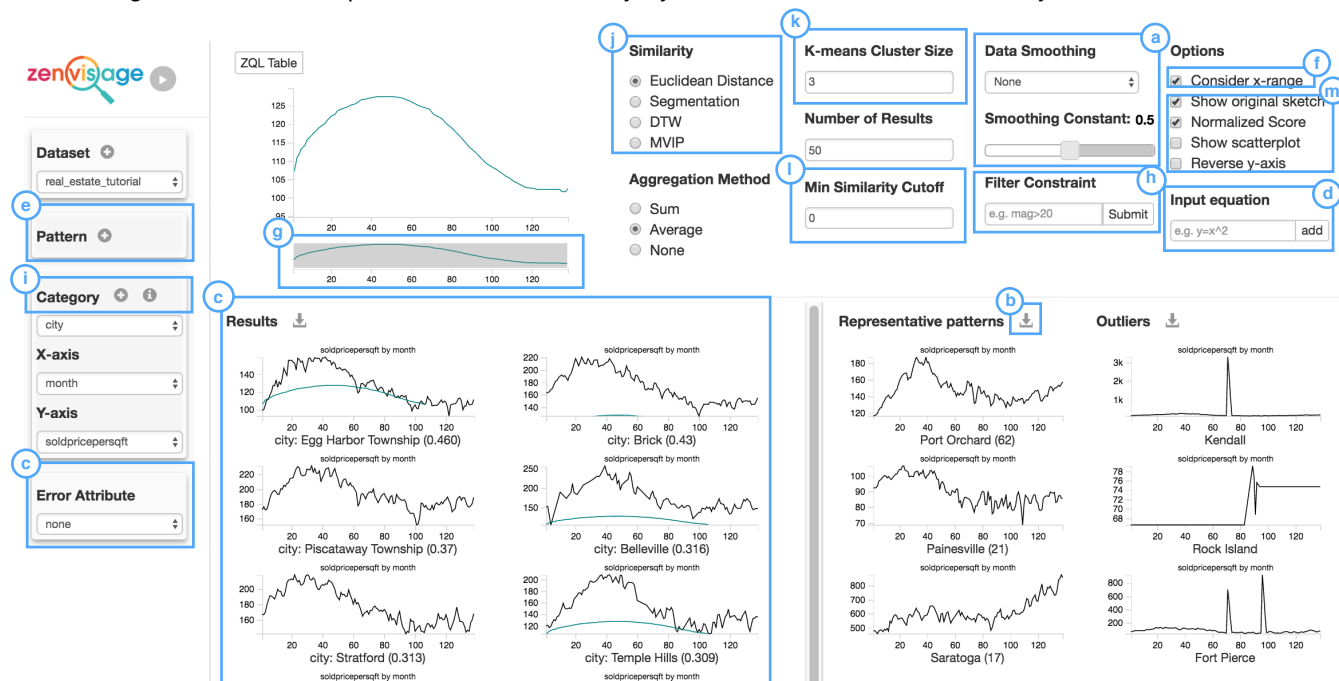


Figure 3: Our VQS after participatory design, which includes: the ability to preprocess via (a) interactive smoothing; (b, c) the ability to export data outputs ; querying functionalities via (d) equations and (e) patterns; query specification mechanisms including (f) x-range invariance, (g) x-range selection and filtering, (h) Filtering, and (i) Dynamic class creation; (j, k, l) system parameter options; (m) visualization display options. Prior to the participatory design, *zenvisage* only included a single sketch input with no additional options. *zenvisage* also displayed representative patterns and outlier patterns, as shown in Figure 1.

Increasing expressiveness of querying capabilities

While the interactions in our original prototype enabled simple visual queries, many scientists were interested in extending their querying capabilities, either through different querying modalities or through more flexible query specification methods.

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 5d).

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 5e). 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 feature. G1 also expressed that she does not really know what is the “trigger point” of when the expression level of a gene will rise and it would be interesting to find all “rising” profiles independent of the change-point. We implemented an option to ignore the x-range in shape matching (Figure 5f) and a brushing mechanism that enables users to select the specific x-region they want to perform their shape matching on (Figure 5g).

Ability to dynamically facet through subsets

Past studies in taxonomies of visualization tasks have shown that it is important to design features that enable users to select relevant subsets of data in visual analytics[2, 9]. We designed two dynamic faceting features coupled with coordinated views that enabled users to specify subsets of data they are querying on and see immediate changes updated in the query, representative, and outlier results.

Filtering Constraints: Users with large datasets first used their domain knowledge to narrow down their search to a subset of data. This would increase their chances of finding an interesting pattern for a given query. To filter data, users could submit one or more SQL-like WHERE conditions as filter constraints in a text field (Figure 5h).

Dynamic Class Creation: In order to address material scientists' needs for creating subsets (or classes) of data on-the-fly to make comparisons between them, we implemented dynamic class creation. This feature allows users to bucket data points into customized classes based on existing properties, and subsequently allows users to compare between the customized classes. For example, the scientists can create three different classes based on a single property alone: Solvents with ionization potential under -10 kJ/mol, over -8 kJ/mol, and ones that fall between -10 and -8 kJ/mol. Then, they could browse how the lithium solvation energy differed for the three custom classes.

Scientists can utilize multiple properties to create custom classes, effectively slicing-and-dicing the data based on their needs. The information regarding the created classes is displayed in the dynamic class information table or as a tooltip over the aggregated visualizations, as shown in Figure 4.

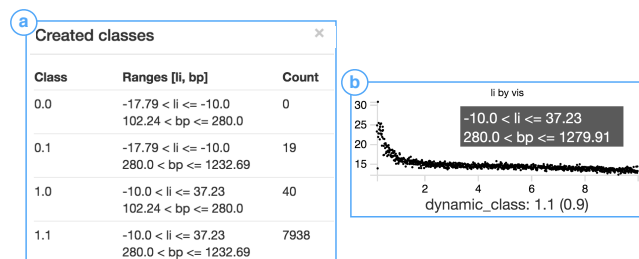


Figure 4: Example of dynamic classes. (a) Four different classes with different Lithium solvation energies (li) and boiling point (bp) attributes based on user-defined data ranges. **(b)** Users can hover over the visualizations for each dynamic class to see the corresponding attribute ranges for each class. The visualizations of dynamic classes are aggregate across all the visualizations that lie in that class based on the user-selected aggregation method.

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 [4, 22].

Controlling VQS internals: 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. [5], 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 5j), the cluster size in the

representative patterns (Figure 5k), setting a minimum similarity threshold for displaying the search results (Figure 5l), and the ability to tune the smoothing algorithm and parameter (Figure 5a).

Displaying interpretable explanations for VQS recommendations: 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 (Figure 5m). We further provided display-related options for plotting modifications, including displaying error bars, and toggling between a scatterplot and line chart view, to help analysts better understand the visualizations.

6 DESIGN GUIDELINES

Search-Browse Paradigm

Top-down approaches

Bottom-up approaches

7 CONCLUSION

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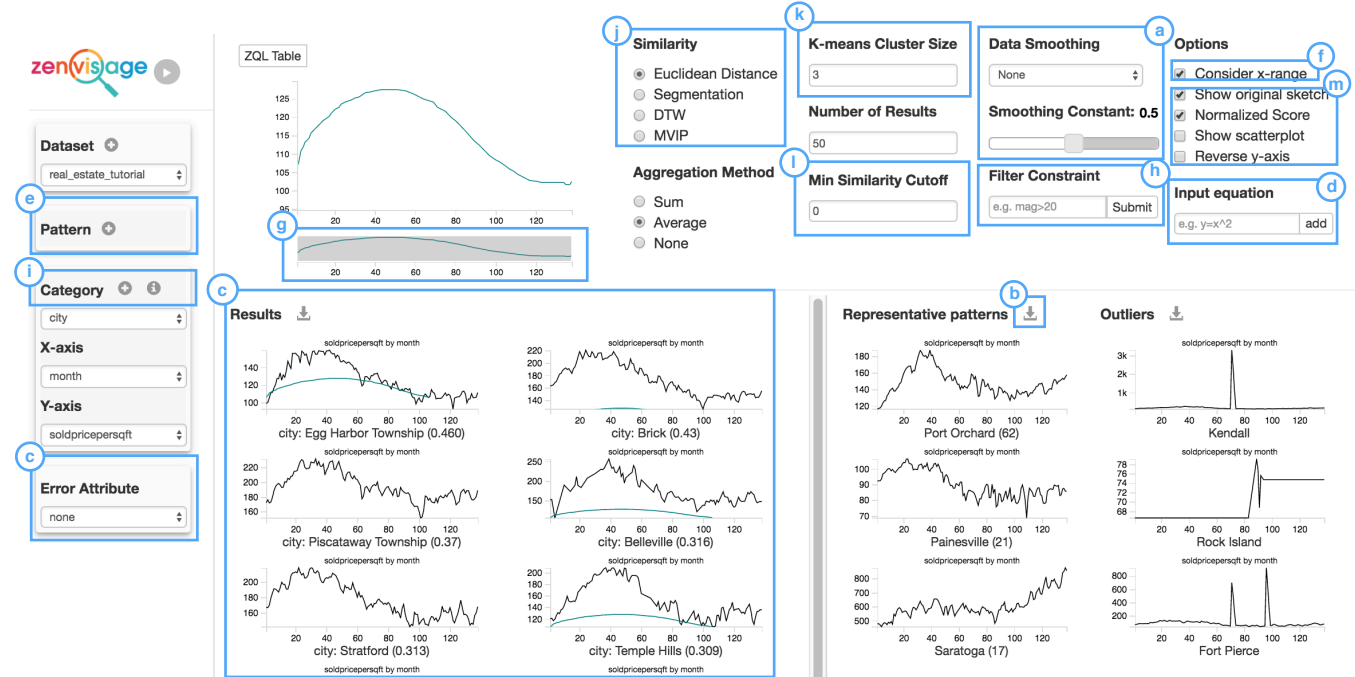


Figure 5: Our VQS after participatory design, which includes: the ability to preprocess via (a) interactive smoothing; (b, c) the ability to export data outputs; querying functionalities via (d) equations and (e) patterns; query specification mechanisms including (f) x-range invariance, (g) x-range selection and filtering, (h) Filtering, and (i) Dynamic class creation; (j, k, l) system parameter options; (m) visualization display options. Prior to the participatory design, *zenvisage* only included a single sketch input with no additional options. *zenvisage* also displayed representative patterns and outlier patterns, as shown in Figure 1.

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