Loops: Leveraging Provenance and Visualization to Support Exploratory Data Analysis in Notebooks

Klaus Eckelt, Kiran Gadhave, Alexander Lex, and Marc Streit

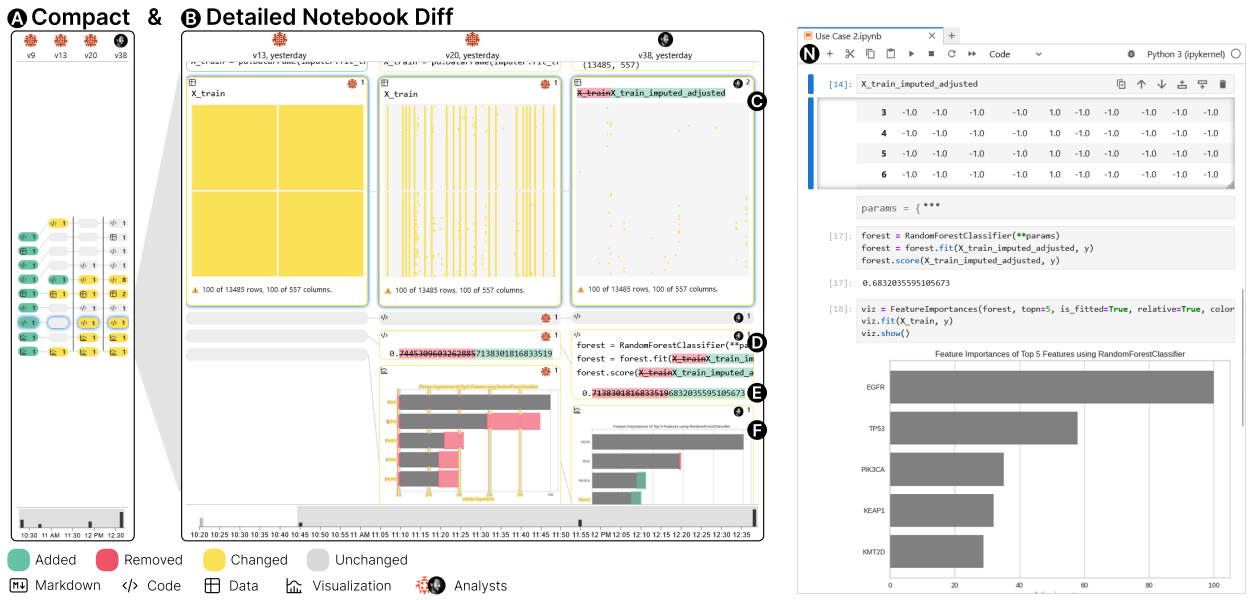

Fig. 1: A Loops enabled notebook showing the evolution of the analysis. While the notebook N only shows the most recent state, Loops visualizes the notebook history next to the notebook. The compact notebook diffs A provide an overview of how the notebook's structure and content changed over time. The rounded rectangles represent the notebook cells, color-coded according to their status relative to the previous version. We show the type of cell (markdown, code, tables, visualizations/images) using an icon and show the execution count where appropriate. The detailed notebook diffs B reveal how cell content changed, using difference visualizations specific to the type of content; including tables C, code D, text E, and visualizations F.

Abstract—Exploratory data science is an iterative process of obtaining, cleaning, profiling, analyzing, and interpreting data. This cyclical way of working creates challenges within the linear structure of computational notebooks, leading to issues with code quality, recall, and reproducibility. To remedy this, we present Loops, a set of visual support techniques for iterative and exploratory data analysis in computational notebooks. Loops leverages provenance information to visualize the impact of changes made within a notebook. In visualizations of the notebook provenance, we trace the evolution of the notebook over time and highlight differences between versions. Loops visualizes the provenance of code, markdown, tables, visualizations, and images and their respective differences. Analysts can explore these differences in detail in a separate view. Loops not only makes the analysis process transparent but also supports analysts in their data science work by showing the effects of changes and facilitating comparison of multiple versions. We demonstrate our approach's utility and potential impact in two use cases and feedback from notebook users from various backgrounds. This paper and all supplemental materials are available at https://osf.io/79eyn.

Index Terms—Comparative visualization, computational notebooks, provenance, data science

1 Introduction

Computational notebooks are the tool of choice in many data science applications [11]. As a literate programming tool [36], notebooks combine analysis and narration for the analysis in a single document. Notebooks can integrate diverse formats, such as different programming languages, multimedia content, interactive widgets, and visualizations as part of the output. The most commonly used notebook technology is the Jupyter family [35], the use of which has doubled annually in recent years [50].

The promise of literate programming—interspersing explanatory text with code—is reproducibility of the result. However, previous research has shown that reproducibility is not the norm when using computational notebooks [23, 48, 63, 67]. A large-scale study by Pimentel et al. [48] showed that only 24.11% of 863,878 public Jupyter Notebooks could be re-executed and just 4.03% produced the same results. Computational notebooks "can foster poor coding practices" [47], become messy [24], and as a result, are often not reproducible [23, 48]. Poor coding and documentation practices also affect data analysis reproducibility, as analysts often start with a vague understanding of their resources and goals [3, 26].

The information foraging and sensemaking loop describes how analysts search, filter, and extract information, continuously developing a

- *Klaus Eckelt and Marc Streit are with Johannes Kepler University Linz, Austria. E-mail: klaus@eckelt.info; marc.streit@jku.at.*
- *Kiran Gadhave and Alexander Lex are with University of Utah, United States. E-mail: kirangadhave2@gmail.com; alex@sci.utah.edu.*

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mental model that aligns with the new information and their existing knowledge [49]. In the series of loops that make up the analysis process, each iteration refines the understanding and brings the analyst closer to their goal. But an iterative analysis process does not match well with the notebook's linear structure; hence, it can be difficult for analysts to understand the state of their notebook. For example, analysts often update their code to reflect new insights or hypotheses, losing track of previous attempts and results [54]. Alternatively, they may duplicate their code to compare different approaches, resulting in messy notebooks that contain outdated or redundant code [54, 66]. Another issue, specific to sequentially executed notebooks such as Jupyter, are out-of-order executions that break the logical flow and introduce hidden dependencies [24, 48, 54]. These practices make reproducing the analysis process and results difficult for analysts and others who want to reuse or verify their work.

Previous works tried to mitigate these issues by capturing the provenance of notebooks [33, 55] or providing live support for exploratory and/or iterative data science tasks [15, 16]. However, to date, these two approaches have been studied independently and rarely combined.

To remedy this, we introduce Loops, our **primary contribution**, a novel visual exploration approach that tracks and visualizes the changes of a notebook over time, allowing analysts to better understand the impact of their changes and the notebook's history. Loops juxtaposes the notebook with compact representations of the analysis "loops". Loops visualizes changes made to the notebook and how they impact the output. By tracking the provenance of notebooks and visualizing the history and differences, we can assist analysts in their ongoing analysis by revealing the impact of their changes. We also contribute a discussion of the different types of content found in computational notebooks and how differences in these contents between notebook versions can be effectively visualized. We implement Loops as an open-source JupyterLab extension, available at `https://github.com/jku-vds-lab/loops`. We validate our approach through use cases and feedback from notebook users that demonstrate its utility.

2 Related Work

We start this section by discussing research that studied the prevalent issues of computational notebooks and the challenges analysts face when working with them. We then discuss how the provenance of computational notebooks can be tracked and visualized, followed by existing work on visual comparison aspects.

2.1 Data Science in Computational Notebooks

Computational notebooks support incremental and iterative analyses well, enabling analysts to edit, arrange, and execute small code blocks in "cells". Cells combine an input for code with the output it produces, and can be executed in any order. However, this execution of cells in any order compromises reproducibility.

Large-scale studies document that the order of cells in a notebook and their execution order do not match for more than a third of the notebooks analyzed [23, 48]. In addition, the execution order cannot be tracked by the notebook alone, as only the last state of a cell is visible. In most cases, public notebooks have multiple large gaps in the execution sequence appearing in the notebook, where it is unclear what analysts executed and if it still exists in the notebook [48]. Notebook environments with reactive code execution models avoid issues from out-of-order execution and gaps in the execution sequence as they recompute results when the user changes a cell. Thus, at least the most recent state of the notebook can be reproduced. However, the previous code and outputs are still replaced when changes are made, leading to code duplication and messy notebooks when comparing different approaches. Also, when encountering dead ends, analysts often fail to document intermediate steps [10, 54]. Thus, notebooks are generally unsuitable for documenting the provenance of the analysis process.

Exploring the history of a notebook was rated the most challenging task after deployment in the survey by Chattopadhyay et al. [10]. When asked about remedies for tracking the evolution of a notebook, analysts favored automated versioning of their code and outputs [10]. However, tracking provenance alone is not sufficient. The tracked information must also be easily retrievable and easily digestible, for example, by relating it to another version of the notebook. We conclude that analysts can benefit from techniques that allow them to easily compare visual and textual changes between notebook versions, such as different data versions or alternatives tested [3, 10, 54]. These requirements have guided the design of our approach.

2.2 Tracking and Visualizing Notebook Provenance

In the 2015 UX survey by the Jupyter organization [30], version control was one of the most desired features currently lacking in the Jupyter platform. Traditional version control management with tools like git is commonly used for notebook platforms such as Jupyter and Quarto [51]. However, these document-based notebooks represent visual outputs as encoded strings that frequently change, even if the content does not change, which makes the version history messy and confusing to navigate [10]. Further, traditional version controls cannot track the history of the outputs and metadata, like the execution order, which are not stored as part of the notebook structure.

In the following, we describe related work on tracking and visualizing notebook provenance and what comparisons they allow (compare Appendix). The Git extension for JupyterLab [31], based on nbdime [32], juxtaposes notebooks for comparison and shows differences in code and plain text. Commercial platforms, such as Observable or Google Colab, automatically track changes and store snapshots of notebooks on every change. JupyterLab creates a snapshot every time an analyst saves a notebook. Users can browse these notebook snapshots by date, but they do not provide details about the changes made in each snapshot. In Google Colab, users can also compare the textual content of two selected snapshots, such as code, markdown, or textual output. Comparisons of data or graphical output, including visualizations and images, are not supported. Observable notebooks allow forking to create variations of the analysis, yet lack features for direct comparison or reintegration of changes into the original notebook, which leads to messy workspaces with multiple copies of the same analysis [10]. ProvBook [55] is an extension to Jupyter Notebooks that tracks the provenance of cells. It enables users to compare individual cells to their previous versions by juxtaposing the previous code, the output it produces, and metadata, but without any explicit encoding of the differences. The effect of a change in one cell on other cells is not visible with this approach. MLProvLab [34] tracks the notebook's provenance and displays each version as a graph where the nodes are the notebook's cells and variables are the connecting edges. The graph's evolution over time can be inspected by browsing the executions. From the graph, a cell's code can be compared to earlier executions. MARG [52] visualizes a notebook as a graph with cells as nodes and connects them in the order of the analysis. This way, divergence points in the analyses, after which analysts try out multiple alternatives, can be displayed. The resulting graph is similar to provenance graphs of analysis processes in visual analytics tools [22, 25, 57]. The approach, however, requires manually annotated notebooks and provides no comparisons. AARDVARK [17] is a visual debugging method to identify and compare differences in the program flow and variable values after code modifications. Persist [18] tracks provenance for interactions in interactive outputs in notebooks, yet does not tackle overall notebook provenance.

Most closely related to our work is Verdant [33], which automatically records the provenance of analyses conducted in notebooks and visualizes it in two tabs: the activity and artifacts tab. Like the histories in Google Colab and Observable, the activity tab lists time-stamped revisions. For each revision, a barcode visualization summarizes the changes to the notebook. Selecting a revision opens the notebook's old state in a separate tab in JupyterLab. Verdant's artifact tab lists the cells and displays the input and output versions. Analysts can inspect the history of cells across all notebook revisions. In all views, only differences in the cell's code input are highlighted.

In contrast to the works described above, our visual representation of the notebook and its history resembles that of the source notebook. Instead of representing the notebook with a graph or barcode, we

represent the notebook cells as rectangles aligned from top to bottom next to the notebook. In addition, we align the history with the cell that is currently active in the notebook. Loops' visualization of the notebook history shows the notebook structure, how it changes over time, if and how the cells have changed, who changed them, and summarizes the difference between the various types of content in the notebook, thereby providing a comprehensive view of the changes made.

2.3 Visual Comparisons

Comparison of different states of inputs and outputs is an essential task for understanding the evolution of notebooks. However, the types of content present in notebooks are diverse, and hence, efficient comparison methods have to be tailored to the type of content. This section discusses ways to compare notebook content visually, focusing on plain and rich text, code, data tables, and images. We do exclude dynamic content such as audio, video and embedded websites.

Gleicher et al. [20] describe the design space of comparative visualization as being made up of *juxtaposition*, *superimposition*, and *explicit representation*. *Juxtaposition*—presenting objects side-by-side or over time through animation—is often easy to implement and can be used for any visual representation. The downside of the approach is that it relies on memory for comparison. *Superimposition*—placing objects in the same coordinate system—is common for spatial data or comparisons of similar objects but can easily lead to clutter. *Explicit representation* directly encodes differences, eliminating the need for mental comparisons. To contextualize differences, explicit representation is frequently combined with superimposition or juxtaposition. In the following, we discuss visual difference encodings for the various content types present in notebooks.

Text difference visualizations are widely employed in text editors. Overleaf and Google Docs, for example, track and highlight textual changes for plain and rich text. Myers algorithm [42] is most commonly used to create human-readable text differences. The algorithm computes a "diff" by finding the shortest path in the edit graph for two strings. It is the default option of git and several code editors to show **code differences** [45]. While changes to plain and rich text are commonly visualized within the document with explicit encodings, most code editors default to juxtaposing the compared versions and explicitly encoding additions and removals.We support both in-document and juxtaposed comparison in Loops.

In addition to the layout considerations above, Gleicher [19] also points out that **image differences** could be identified at different abstraction levels: on the data, feature, and image level. The *data* level refers to the raw data to create the image, the *feature* level refers to the abstracted data (e.g., the height of a bar in a histogram), and the *image* level to the resulting imagery. As our approach operates on the visible output of Jupyter notebooks, we focus on related work that compares images (and data visualizations) at the image level.

Notebook environments and the related work discussed so far juxtapose graphical outputs in the notebook, but do not use explicit visual encoding of differences [19]. For superimposition, blending and color weaving have been proposed to combine information from layered images [20, 39]. To explicitly encode differences between images, a common method is to convert them to grayscale and create a difference image by subtracting the individual pixel values of one image from the corresponding pixel values of the other [21, p. 87–90]. Pixel differences can be color-coded, for example, in red and green for negative and positive differences, respectively [27]. However, global translations, antialiasing, or compression in lossy formats can cause large but irrelevant differences [27, 28, 53]. To suppress these artifacts, fuzzy difference methods can be applied that either take neighboring pixels into account [27], or allow a certain distance between the compared pixels in color space [28]. Resemble.js [53] employs a nuanced approach, calculating pixel-based image differences with options to ignore subtle changes, color differences, transparency, and antialiasing; it also provides several modes to visualize differences. VAICO [56] supports comparing more than two images simultaneously, using hierarchical clustering of regions of differences and superimposition of the results.

To identify differences in **data visualizations**, previous studies evaluated the efficacy of superimposition and juxtaposition for various tasks in crowd-sourced experiments [29, 46]. While participants performed best with animated and superimposed visualizations when estimating correlations or identifying the largest difference between visualizations, juxtaposed visualizations performed better for certain tasks [29]. Vis-a-Vis [6] visualizes the evolution and differences in visualizations in the context of changes in code and code structure. Vis-a-Vis displays the current source code, output, and a revision tree, grouping revisions by code structure. The interface displays outputs linked to a structure, along with a comparison image showing the outputs' per-pixel variance. In Loops, we juxtapose or superimpose two images (including images of data visualizations) and highlight pixel differences. We color-code pixel differences to indicate added, removed, or changed content. We also group neighboring changes by slightly dilating the pixel-based difference. If the images/visualizations are superimposed, we provide sliders to vary the opacity of the images dynamically.

As data is fundamental to data science, **data differences** are at least as important as code differences. Datasets evolve over time as analysts filter, clean, update, or expand them during their work. However, data difference visualizations are rarely integrated into the tools used by analysts. While notebooks can be used to analyze arbitrary data set types, we focus on arguably the most common data type: tabular data. TACO [44] introduces an approach to visualizing changes in data tables. The technique categorizes changes as additions and removals, merges and splits, reorders, and content changes. TACO juxtaposes the compared tables and shows a heatmap of the differences, highlighting content modifications, additions, and removals through distinct colors. Furthermore, the changes are summarized in a histogram, offering an overview of each version. CHAMELEON [26] visualizes the impact that changes in data have on machine learning projects. It shows a data version timeline, from which two versions can be compared.

Superimposed diverging histograms visualize data distribution changes and the impact on the machine learning model's predictions is shown through a sensitivity histogram and a prediction change matrix. In prior work [14], we visualize data sets that change over time as time curves [4]. Juxtaposed summary visualizations and explicit difference visualizations show how the data changed between two versions, with differences sorted based on the extent of change. Perhaps most closely related to our work is Diff in the Loop [61], which contains a code editor that tracks changes to code and runtime variables. A separate view shows how the data set has changed through code edits by visualizing the distribution of all affected features.

In Loops, we explicitly visualize the differences in tabular data by color coding changes, additions, and removals. The resulting visualization is similar to the heatmap in TACO [44]. However, we do not incorporate color coding to indicate the magnitude of change within a table's cell, nor do we consider the reordering of columns a change. The effects that differences of the tabular that have on the subsequent analysis are not visualized directly but through the difference visualizations in the following cells as soon as they are re-executed.

3 Loops Approach

Data analysis is an iterative process. Based on the insights analysts gain during their analysis, they need to change their previous code and assess how the results are affected. With Loops, we not only track the notebook provenance to document the analysis, but also to support the ongoing analysis process. We aim to achieve this by visualizing how the notebook has changed in the series of loops that make up the analysis process. We show the changes made by analysts and their impact on the notebook outputs with difference visualizations (*diffs*) for the whole notebook and individual cells.

Loops design is guided by the issues that analysts face when working in notebooks (see Sec. 2.1). First, we help analysts document their analysis process, including all intermediate steps, by automatically recording the notebook's provenance. Second, exploring the history of a notebook was rated as one of the most challenging tasks [10]. We remedy this with Loops notebook history visualization, which reveals when and in what order cells were changed and executed, which cells were changed most frequently, and whether other collaborators have

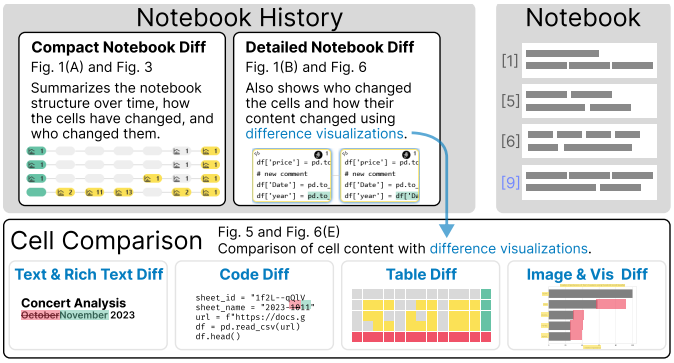

Fig. 2: The notebook's history is presented next to the analyst's notebook, visualizing changes between notebook versions with compact or detailed notebook diffs. The cell comparison can be opened on demand to explore the differences in further detail.

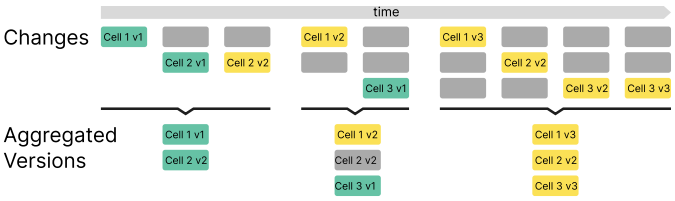

Fig. 3: Aggregation of notebook changes to the versions visualized with Loops. Each column of changes corresponds to an execution of a cell. Instead of a temporal aggregation, we merge all changes into one version as long as the notebook is executed from top to bottom. Note that no information about the structure of changes is lost.

changed any cells. We summarize all this information for individual notebook versions in the compact notebook diff. A detailed notebook diff also reveals how cells were changed, addressing the third issue analysts face in notebooks: comparing alternatives. Currently, comparisons happen by duplicating code, resulting in notebooks with outdated or redundant code [54]. We facilitate the comparison by placing the notebook history next to the notebook and aligning the diffs in the history with the currently active cell in the notebook (see Fig. 2). The detailed notebook diff shows difference visualizations for every change in the cells' input and output. This allows us to show the changes made by analysts, but also the impact of their changes on other cells. Loops also provides a full-width detail view for cell comparison, with which individual changes can be explored further (see Fig. 2).

In the following subsections, we explain how Loops tracks the notebook's provenance and how it is visualized and compared in its components. The supplementary video (see Sec. 8) demonstrates the workflow and interactions.

3.1 Tracking and Visualizing the Notebook History

Loops automatically records the interaction provenance, as requested by analysts in prior work [10]. Every time users execute a cell in the notebook and thus update it, Loops saves the notebook's state. Loops stores the cells of the notebook, their order, which cell was active and executed, who executed it, the cells' input (i.e., the code) and output, and how these inputs and outputs were displayed in the notebook–rather than the content of variables used in the execution. Consequently, Loops stores everything an analyst sees while working in the notebook and thus influences their information-foraging and sensemaking loops. The goal of Loops is not to collect comprehensive provenance that guarantees reproducibility but to support and make the iterative analysis process comprehensible. We argue that through this support, many challenges analysts face when working with notebooks can be mitigated (see also Sec. 1).

As with most provenance data, the scale of interaction histories can become uninterpretable and overwhelming quickly [10,57]. Therefore, we considered how the provenance can be best aggregated. If at all, previous work grouped notebook versions by temporal proximity (see Appendix). For Loops, however, we decided to take a different approach that leverages the semantics of notebooks: We group the stored notebook states as long as their cells are executed in linear order, i.e., from top to bottom, even if the analysis is interrupted (see Fig. 3).

Although the analysis process is typically not linear, its steps still build on each other: Data must be loaded before exploration, cleaned before modeling, etc. These dependencies are also reflected in the structure of the notebook [52]. Going back in the notebook—and re-evaluating already executed parts—corresponds to a new iteration of the analysis loop. In Fig. 1 A, for example, a new version is introduced as the analyst edits and re-executes the first cell of the notebook again before updating the data processing step and re-running the modeling step with the new data. The aggregated notebook provenance thus reflects the analysis loops we visualize and compare in Loops.

This methodology to record and aggregate the provenance of notebooks is designed primarily to address the challenges encountered in sequentially executed notebooks (see Sec. 2.1). However, we argue that our approach is also valuable within reactive notebooks (see Sec. 7).

The versions are visualized and arranged horizontally according to their creation order. Each cell is represented as a rectangle with rounded corners, reminiscent of a notebook cell. Like in a notebook, the cells are arranged vertically. Cells of adjacent versions are connected by thin gray lines, which serve as a visual guide for tracing cells across the notebook's versions. This is especially helpful if cells are not aligned due to different content, representation, or ordering (see Fig. 4). In addition, we align the cells of each visualized version around the cell that is currently active in the notebook. When the analyst changes the active cell, our provenance visualization re-aligns the cell's history vertically to enable better comparison (see Fig. 6 E).

Notebook versions can be visualized at two levels of detail: (1) The compact notebook diff provides an overview of the version, indicating added, changed, executed, and deleted cells. (2) The detailed notebook diff also reveals the cells' content and changes compared to the previous version. Below the notebook diffs, Loops displays a bar chart with a continuous time scale showing the temporal distribution of the notebook versions and the extent of their changes, indicating active and dormant periods of the analysis (see Fig. 4). By visualizing the structure of the notebook, how and when it changed, and who changed it, we address the analysts' need for a retrievable and comparable history [10].

3.1.1 Compact Notebook Diff

The compact notebook diff, shown in Fig. 4, gives an overview of the evolution of the notebook, showing all cells in the same small size. We embed icons that indicate whether a cell contains markdown or code. If a code cell produces outputs, we encode the output type, i.e., whether it is a table or a visualization. Furthermore, an execution counter displays how often the cell was executed in each version. This helps identify the parts of the notebook that have been modified the most or not executed at all. Cells are color-coded according to their status: unchanged, changed, added, or deleted relative to the previous version. In accordance with common comparison tools for text and code, we use color-blind safe shades of green and red for additions and removals, yellow for content changes, and gray for unchanged content. Furthermore, the currently active cell in the notebook is emphasized with a blue shadow (see Fig. 4). When multiple analysts contributed to a notebook, we indicate each version's contributors at the top of the difference visualization (see Fig. 4). Contributors are sorted according to the number of executions they performed.

The compact cell design allows us to display 30 cells on Full HD screens without scrolling. This allows us to present the majority of notebooks in their entirety, as prior research indicates that more than 50% of all notebooks comprise 30 cells or fewer, and 95% contain 100 cells or fewer [54]. Fig. 4 shows an analysis carried out over several weeks with 211 executions visualized in 27 versions.

3.1.2 Detailed Notebook Diff

The detailed notebook diff, shown in Fig. 1, visualizes the changes in both code and output of a cell, allowing analysts to understand their

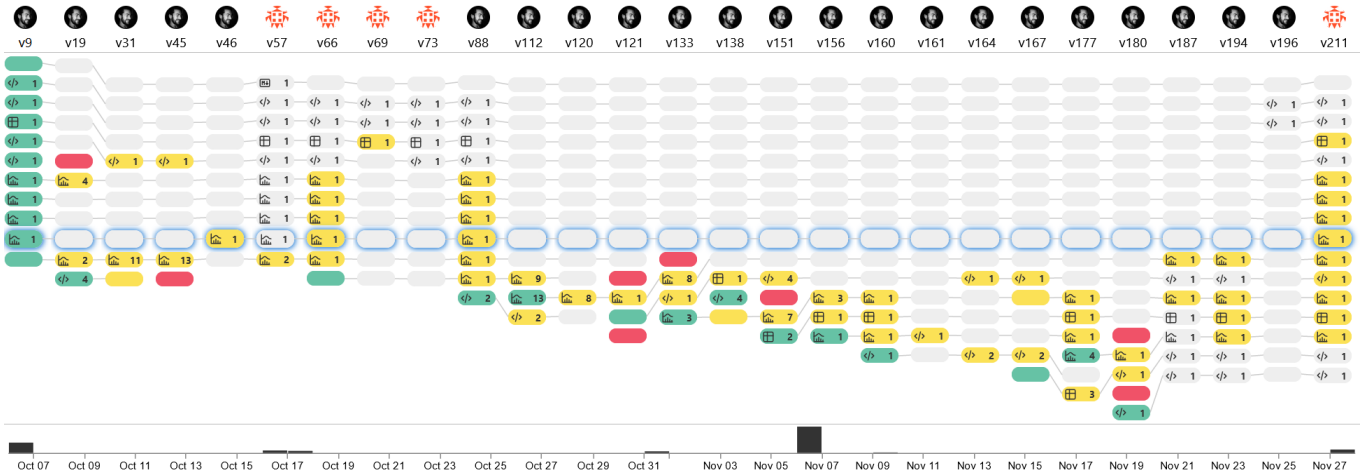

Fig. 4: Notebook history with compact notebook diffs for an analysis conducted over several weeks. Rounded rectangles represent the notebook cells, which are color-coded to show insertions (green), removals (red), change (yellow), and no changes (gray). For executed cells, we show how often each cell was executed plus an icon indicating whether the cell contains markdown or code. For code cells, we change the icon if the cell outputs a table or visualization. The cells of the versions are aligned around the active cell, emphasized with a blue shadow In the initial version on the left, the first analyst created and executed multiple cells. Later, mainly the cells at the end of the notebook were edited iteratively, and the entire notebook was executed again only a few times, after the analyst changed in versions 57, 88, and 211.

changes' impact better. We adapt the displayed cell content depending on its output and change to give a better overview of a notebook version.

The content of markdown cells with headlines and code cells that output visualizations or images are always shown, as these elements provide structure to the document, and showing them facilitates navigation [10,54]. However, we limit the cell content shown to the markdown cells' headings and the code cells' visualizations/images, as long as other cell parts are unchanged. If there are no changes, code or outputs that don't generate a visualization have their content hidden. Cells where neither the code nor the output are displayed are represented with a small rectangle, as in the compact notebook diff. This approach allows the notebook diff to focus on changes and their impact across the notebook (see Fig. 1 B). If there are changes in code or outputs, a superimposed difference visualization for the respective cell content is displayed (described in Sec. 3.2). The code and the outputs of the currently active cell are always displayed so that the history of the cell can be easily tracked and compared, as illustrated in Fig. 6 E. Because we display the content of cells in the detailed notebook diff, we shift from color-coding the entire cell to color-coding only the cell border. This adjustment addresses contrast issues and ensures the cell content remains clearly visible.

In addition to its content, we show the cell's type and how often it has been executed in the top left and right corner, respectively, mirroring the compact notebook diff. Furthermore, we show who contributed to the changes in the cell. Contributors are represented by avatars adjacent to the execution count and are arranged based on the number of executions they have performed (see Fig. 1).

3.2 Visualizing Cell Content Differences

For a comprehensive comparison of the cell content, analysts can open a separate detail view for cell comparison from each cell in the history. We show this view below the notebook to leverage horizontal space that is useful for side-by-side comparisons (see Fig. 6 C).

The cell comparison can be used for either code or output and features large difference visualizations that display the content of the cell and how it changed (see Fig. 5). The view automatically shows an appropriate difference visualization based on the content type. We have carefully designed visual encodings that consistently visualize changes in the cell's code and the various types of content present in the cell's output. All difference visualizations can display either juxtaposed or superimposed comparison, offering flexibility in viewing and comparing changes. In both layouts, changes are explicitly encoded by applying the same color scale used for cells.

Next, we introduce the difference visualizations tailored for various content types. These visualizations are employed not only in cell comparison but also in the detailed notebook diff, albeit in a more condensed format.

3.2.1 Text and Code Comparison

For the visualization of text and code differences, we based our designs on standard methods used in word processors and editors. Our difference visualization employs the Myers algorithm [42], which is widely used to detect insertions and deletions in text. Myers difference algorithm is particularly effective for comparing text documents, as it can efficiently identify the longest common subsequence of words or lines between two texts, making the display intuitive to understand. We use this approach for plain and rich text.

For visualization of code differences, we use a dedicated code editor. This editor provides syntax highlighting and employs the Myers difference algorithm but with additional post-processing steps applied to the detected changes (see Fig. 5 A). These additional steps account for the unique characteristics that code presents in contrast to text documents to ensure that the differences are meaningful and relevant. Alternative algorithms have been shown to provide better results for code than the standard Myers algorithm, but prior work has not considered post-processing steps [45]. Given its frequent use in coding tools and developers' ensuing familiarity, we chose this combination over alternatives.

3.2.2 Tabular Data Comparison

Understanding how tabular data changes over the course of an analysis is crucial. Changes may be introduced through code or updates of the data source [3,26,41]. In Loops, these changes are explicitly visualized. Inspired by TACO [44], our visualization compares two tables as they are output in the notebook. It identifies changes within the cells of a table and also detects the addition or removal of rows and columns. Columns or rows that are added or removed are highlighted in green and red, respectively. Changing the order of columns is not considered a change, as the columns' data remain unchanged. Cells in a table with changed content are highlighted in yellow; removed or newly added content is juxtaposed within the cell, with the removed text being struck through (see Fig. 5 B).

3.2.3 Comparing Images and Visualizations

Images and data visualizations can be compared at multiple levels: on data, feature, and image level [19]. In Loops, we compare them at the image level (and assume visualizations are rendered as raster graphics)

Fig. 5: Detailed code, table, and data visualization differences. The code difference Ⓐ shows that the plotted subset was extended and that the data for the visualization's *x* and *y* axes were preprocesed further. The table difference visualization Ⓑ shows that the concert data's price column was adjusted and a empty column was added. The data visualization difference Ⓒ shows changes in the y-axis labels and regression lines.

and thus do not differentiate between images and data visualizations in the following. While the comparison is made at the image level, the image difference visualization is part of a broader context that includes differences of all other steps preceding the image change. The difference visualization we propose aims to highlight smaller changes in particular, as larger changes—such as changes to the underlying data, the plot type, or one of its encodings—are also reflected in the data or code differences. The Appendix contains a gallery of difference visualizations for several types of visualizations and changes in them.

Balancing the needs for comparison between generic images (photos, diagrams) and data visualizations is difficult. For instance, a slight change in brightness may not matter in a photograph but can indicate a crucial change to the data underlying a heatmap. Given the data science focus of this work, we prioritize the requirements for comparing data visualization over those for generic images.

Image subtraction is used routinely for enhancing differences between images [21, p. 87] and is useful when changes in successive images need to be detected [9, p. 429]. This is the primary use case of our work: to highlight changes between iterations. We use pixel-based subtraction to create the difference visualizations for images. The process is illustrated in the Appendix.

If the image sizes vary, they are first scaled, preserving their aspect ratio, and subsequently padded to the same size. We pad to the right and top because data visualizations usually align axes with the bottom left. To determine the color for the added pixels as part of the padding process, we extract the background color by analyzing the outermost 1% of pixels on all four borders of the image, and assume that the most frequent color is the background color. The images are then subtracted and subsequently turned into grayscale by calculating the perceived luminance of each pixel to preserve the color differences [9, p. 256]. Thresholding converts the grayscale image into a binary image, by setting all pixels exceeding a 1% change in luminance to white (changed) and all others to black (unchanged). As the pixel-based approach may result in many small disjoint changes, we apply additional morphological operations to make the difference visualization more comprehensible, akin to summarizing text changes on a word rather than a character level. Differences are dilated twice, which merges adjacent differences into one, using a 3×3 kernel for the detailed comparison and a 9×9 kernel for the detailed notebook diff to ensure visibility in the scaled-down representation. Afterwards, the differences are eroded once, using the same kernel, to reduce the size of the differences again. Performing the erosion only once (when we dilated twice) results in the difference being slightly larger than the changed content, forming a small border around the changed pixels. This approach is inspired by the background color used to mark changes in text, providing a clear and distinct visualization of modifications (compare Appendix). The calculated difference is then transformed into an RGB image. Pixels that changed from the background color to a different color are encoded in green, from a non-background color to the background color in red, and pixels that changed color in yellow (see Fig. 6 Ⓔ). Our algorithm has a linear time complexity with respect to the image size ($O(n)$). We also calculate the changes' bounding boxes. In initial experiments, we highlighted changes using rectangular or convex hull bounding boxes, but within the bounding boxes the changes were challenging to identify. Instead, we now count the bounding boxes to inform the user about the number of changed regions in the image, first removing any bounding boxes nested within others, to highlight subtle changes as in the scatterplot in the Appendix.

Users can choose whether the images with explicit difference encoding are displayed juxtaposed or superimposed. In the superimposed difference visualization, the images are combined with alpha blending, and the opacity levels can be controlled with a slider (see Fig. 5 Ⓒ).

Whether juxtaposition or superimposition is better is task-dependent [20, 29, 46]. Generally, superimposition is most helpful if the compared images are similar, while significant changes are better represented in juxtaposed views [20, 29, 46]. We therefore superimpose highly similar images and juxtapose dissimilar images. To determine similarity and decide on the layout to use by default, we evaluated multiple image similarity metrics: (*i*) Mean Squared Error (MSE), (*ii*) Structured Similarity Index (SSIM) [64], (*iii*) Normalized Mu-

tual Information (NMI) [58], and (*iv*) Oriented FAST and Rotated BRIEF (ORB) [8]. We excluded MSE and NMI from further consideration due to a lack of interpretability of the resulting value. The results of SSIM and ORB are promising, but to avoid a discrepancy between the visualized differences and the calculated similarity we opted for a more straightforward approach based on our explicit encoding of differences. We divide the number of changed pixels by the total number of pixels in the image to obtain a relative pixel similarity measure. Further details on the similarity metrics and the results of our experiments are provided in the Appendix.

In addition to guiding the default representation (superimposed vs juxtaposed), we also show the numerical value in the difference visualization. We present the difference visualization superimposed as long as the similarity is at least 90%. Otherwise, we use the juxtaposed layout. If the similarity of pixels is less than 80%, we remove the explicit encoding of differences, assuming that the images are different enough to be recognized without visual aids. Our experiences match findings by Lyi et al. [38] who found that "explicit-encoding can be used for designs where visualizing subtle difference is of importance".

4 Implementation

We have implemented the open source prototype of Loops as an extension for JupyterLab that is available on GitHub: `https://github.com/jku-vds-lab/loops/`. A deployed instance of JupyterLab with Loops is available at: `https://mybinder.org/v2/gh/jku-vds-lab/loops/main`; this instance also contains example notebooks. Although the screenshots and use cases presented in this work use Python, the Loops prototype can be used with any programming language available in Jupyter, as it only operates on Jupyter's frontend and has no dependencies on the notebook's kernel.

We use Trrack [12] to store the notebook states as a provenance graph. For the difference visualizations, we use html-diff [59] for rich text differences, the Monaco Editor [40] for code differences, D3 [7] for table differences, and OpenCV [8] for image differences.

5 Use Cases

We demonstrate Loops by means of two use cases. The first use case presents an analysis of Austrian concert data conducted over several weeks and demonstrates Loops' visualization of the analysis history. The second use case demonstrates how we support analysts in comparing the results of a what-if analysis on data from lung cancer patients. The notebooks of the two use cases, together with the provenance of the analysis, are available in the deployed instance of Loops: `https://mybinder.org/v2/gh/jku-vds-lab/loops/main`. Furthermore, we collected qualitative feedback from notebook users with various backgrounds, which we summarized in Sec. 6.

5.1 Use Case 1: Multi-Week Concert Data Analysis

Our use case presents an analysis of Austrian concert data conducted over several weeks and demonstrates Loops visualization of a long analysis by two analysts (see Fig. 4). The data set is a long-form table with 501 entries from 2003 to 2023, describing the artist, date, location, ticket price, and act (headliner/support). We load the concert data from an external Google Sheets spreadsheet, which is updated regularly and allows us to show differences that are not caused by code changes. The history contains 211 executions represented in 27 versions. The final notebook consists of 16 cells, a typical size for notebooks [54].

Analyst starts the analysis on October 6th by importing the concert data and applying a few initial data wrangling steps. They then profiled the tabular data to examine available years and how distributions change over time. The primary goal of the analysis was to investigate the increase in ticket prices over the years. While they created various plots using different visualization techniques, it was necessary to repeatedly return to the data wrangling step to update the data types to fit the plot (v19–v46 in Fig. 4). After updating the data, the visualization cell was changed up to 13 times in one version.

The analyst re-executed the notebook on October 16th (v57) and 17th (v66). The detailed notebook diff reveals no code changes, but outputs were changed due to external data updates. As cell outputs are overwritten upon execution, investigating how an output changes with new data becomes challenging, particularly with multiple outputs in the notebook. In this context, **Loops enhances our ability to recognize and track changes by clearly highlighting output differences.**

The most extensive phase of the analysis occurred on November 6th, involving 118 of 211 versions, visible in the bar chart in Fig. 4. Analyst extended the visualization of price trends over time with regression lines and adjusted prices for inflation by including a data set containing inflation rates. Adjusting prices for inflation required several iterations, and **we used Loops to verify the changes using the difference visualizations** shown in Fig. 5. In the last version of the notebook from November 27th (v211), analyst executed the entire notebook, which caused the visualizations to change due to the updated concert and inflation data.

The history of the notebook shown in Fig. 4 provides several insights: (1) The first analysis steps by analyst are represented in the first five versions of Fig. 4 that summarize 46 notebook versions. They show that after creating and executing the cells with basic visualizations of distributions, most changes and executions aimed at visualizing the price trend. This involved repeated cycles of changing the data format and visualizations. (2) Versions in which we resumed the analysis after a break are evident as the notebook was re-executed from the top, ensuring that required libraries and the data are loaded. This can be seen in versions 57, 66, 88, and 211 of Fig. 4 that correspond to October 16th, 17th, November 6th, and 27th, respectively. (3) Versions 57, 88, and 211 additionally indicate a transition to a different analyst. (4) The history also shows that during the extensive analysis on November 6th (v88–v194), no changes were made to previously created cells.

5.2 Use Case 2: What-If Analysis on Cancer Patient Data

The analysis in this use case builds on our previous work comparing lung cancer patient cohorts from the AACR Project GENIE [1, 13]. We aimed to validate the mutational differences between these cohorts, as reported in the literature [43]. However, we found that the cohort data also considerably varied in the amount of missing data. Our approach identified mutations in the FGFR4 gene as a key feature to differentiate between patient cohorts, although they differed primarily by the amount of missing data. We hypothesized that this gene would have minimal impact if the data were complete. In this analysis, we now want to go beyond the available data and perform a what-if analysis, substituting the missing data [37].

The first analyst begins by replicating our previous findings. They import the necessary libraries, load the cancer patient cohort data, and inspect the data set. As the goal is to identify differences between cohorts using a random forest model, they separate the features used for the prediction and the cohort labels into distinct variables. They perform basic feature selection, eliminating features with the same value for all patients, as these do not provide any information for our model. After this, they again inspect the data set to verify the changes. They also create a visualization to show the distribution of FGFR4 genetic mutations among the analyzed cohorts. After preparing the data, they set hyperparameters, train the random forest model, and output its accuracy. They create a bar chart to visualize the model's most important features, and the results align with our previous analysis.

Next, the analyst substitutes the missing data and assesses how the results of the analysis change. They extend the initial feature engineering step and substitute the missing genetic data with a nearest-neighbor approach using the data of the five patients with the most similar genetic profile (Fig. 6 B). As they output the new data, all of the cells are marked as changed (Fig. 6 C), due to a change in data type by averaging the nearest neighbors data. They therefore change the code to only use the data of the most similar patient (Fig. 6 D). After re-executing the subsequent cells, the detailed notebook diff shows that the bar chart changed significantly for the new model. The analyst opens the cell comparison (Fig. 6 E) and sees that FGFR4 is no longer one of the most important features distinguishing cohorts. Also the overall order of important features has changed significantly, as highlighted by the bars' altered labels. EGFR now ranks as the most significant gene, followed by TP53 and PIK3CA. KEAP1, and PTPBR have been added

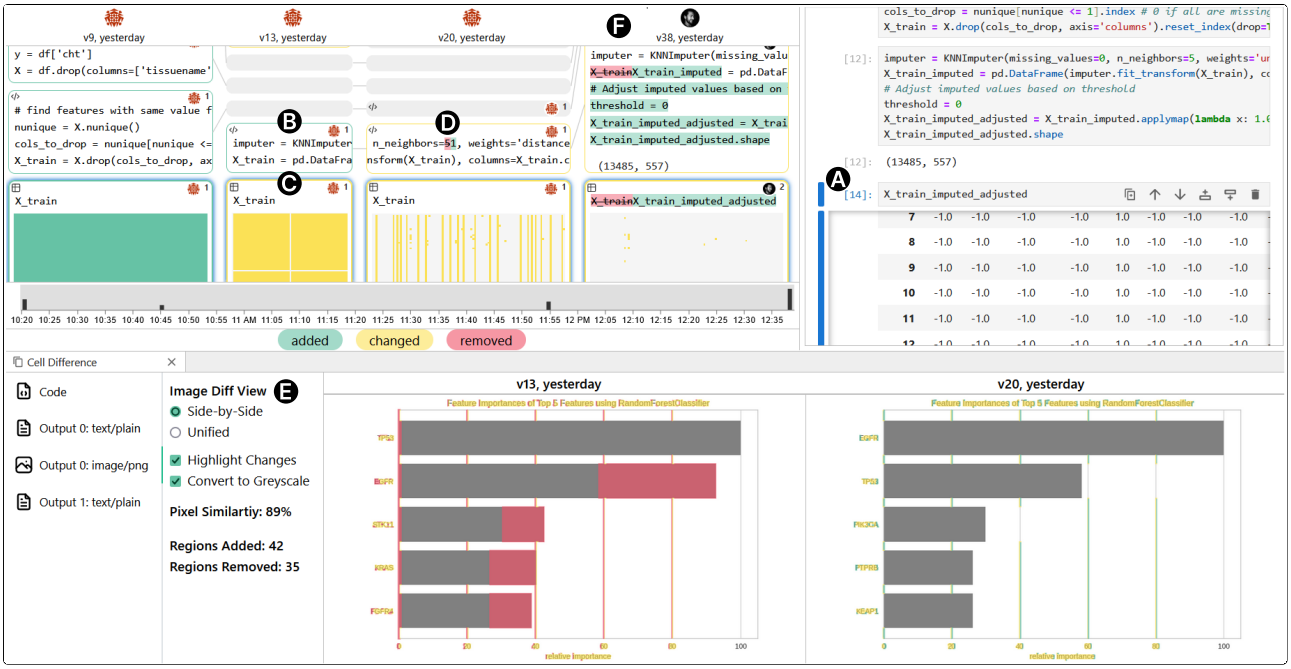

Fig. 6: Analysis of cancer patient data in JupyterLab with Loops. The cells in the notebook history are aligned with the currently active cell in the notebook Ⓐ. The visualization of the notebook's evolution shows four versions corresponding to the initial execution of the notebook and the following what-if analysis. Analyst adds a cell to substitute missing values Ⓑ, which changes the data Ⓒ. They subsequently update the code in version three Ⓓ and retrain the model with the new data, which changes the features that are most important to distinguishing cohorts Ⓔ. Analyst then updates the code for substituting missing values again in the final version of the notebook Ⓕ.

to the list, while STK11 and KRAS have been removed (Fig. 6 Ⓔ). In the last version of the notebook (Fig. 6 Ⓕ), another analyst reworked the data substitution. They update the code so that the data of multiple patients are considered, as analyst had planned, while keeping the same data type. However, this change results only in minor changes of the data and the model (see Appendix).

This use case illustrates how Loops' difference visualizations can help to identify and assess changes in the outputs, and how Loops facilitates the testing and comparison of different analysis paths. The same procedure can analyze the effects of different substitution methods, models, or hyperparameters. The AACR Project GENIE is an ongoing effort with continuous data updates, so the analysis will need to be repeated in the future. With Loops, any resulting output differences can be quickly identified.

6 Qualitative User Feedback

We conducted interviews to confirm the problems of notebook users described in Sec. 1 and Sec. 2 and to gather expert feedback on Loops provenance visualization and the comparisons it provides.

6.1 Participants

We gathered feedback by interviewing notebook users with various backgrounds: a student (S) in AI, a professional data scientist (DS) in marketing, a researcher (R) in human-centered AI, and a lecturer (L) teaching undergraduate and graduate students in AI. We have two male and two female participants between the ages of 22 and 39 ($Age_{mean} = 30.5$). All participants have a minimum of three years of experience working with notebooks. We recruited the participants from our professional network, targeting individuals proficient in computational notebooks. We emailed invitations to individuals and research groups until we could recruit a representative for each user group.

6.2 Procedure

The interviews lasted 40–60 minutes and were guided by a set of initial questions provided in the Appendix. We encouraged participants to provide think-aloud feedback, fostering a natural conversation flow. Despite this, we ensured that all questions were addressed during the interview. The interviews were conducted individually, recorded, and detailed notes were taken on participants' comments, feedback, and responses. The interviews with DS and R were conducted remotely, while the interviews with S and L were conducted in person. Participants were not compensated for their involvement.

In the interviews, we first asked them questions about how they work in notebooks (see Appendix). As a next step in the interview, we showed them a notebook we had prepared based on the concert data analysis of Use Case 1. We explained the data, the analysis goals, and the notebook structure. We then opened the compact representation of the analysis history. After exploring the compact notebook diff, we started executing the notebook, showing how the history aligns with the currently active cell and how it is updated as cells are executed. We changed the last notebook version to the detailed notebook diff, revealing the changes in data and visualizations. The execution of the notebook with data that have been updated since its last execution (see Use Case 1) resulted in changed outputs. We also opened the comparison detail view for multiple cells to demonstrate the detailed text, code, table, and image difference visualizations.

6.3 Results

Working with Notebooks. Participants S, DS, and R stated that they commonly create multiple cells, each containing code with slight variations to facilitate the comparison of alternatives. When asked how they deal with alternatives once they had picked a solution, none of the participants could articulate the specific criteria they apply. S and DS leaned towards retaining all code, even if it resulted in cluttered notebooks. Notably, all four participants had experienced situations in which they would have needed code they had previously deleted. The four notebook users stated that they mainly work alone on notebooks; collaboration only takes place asynchronously, if at all. These responses are consistent with the results of previous studies [3, 10, 54].

Compact Notebook Diff. Participants stated that the color-coding with green for new and red for removed cells was obvious, yet, they were unsure about the meaning of yellow cells, triggering us to add a legend to Loops. They liked that the cells' execution can be tracked, as they regularly experience issues with out-of-order execution and needed to find out how they got to a particular state. When asked which cells had changed the most, all participants could quickly identify the

corresponding cells. Furthermore, R emphasized the utility of showing a notebook history in collaborative scenarios, allowing users to track changes made after handing over the notebook.

Detailed Notebook Diff. S and DS appreciated how the extension summarizes the individual versions of the notebook. DS added that Loops simplifies analyzing the impact of changes. They also appreciated that the differences are directly visible without using git, and that difference visualizations are available for all content types. R appreciated that previous outputs remain visible, enabling them to revisit them during long-running executions or after unintended executions. They also found the visualization of notebooks and cell content differences intuitive. However, participants also noted some concerns and weaknesses. They expressed a desire to extend the examination of differences beyond the visible contents of the notebook, e.g., to changed variables (R) or to the full data set when it is truncated in the notebook (DS, R, L). L would value the ability to analyze changes from the most recent execution rather than the aggregated changes from the last version of the notebook.

Comparison Detail View. Participant S highlighted the comparison detail view as a great addition to the notebook representation. The participants recognized how the familiar encoding of code differences was translated to other types of content. They consider all difference visualizations to be most useful when changes are subtle. The flexibility to toggle between superimposed and juxtaposed comparisons was also appreciated. For the image difference visualization, DS liked how images are shown in grayscale to highlight the changes with color. S noted that it may surprise her when she sees that a chart has changed significantly, e.g., due to a change in chart type. However, she also added that she could recognize this change based on the differences in the preceding code difference. She also expressed concerns about balancing the size of difference encodings in image difference visualizations for small and large changes. Participant R often creates large composite figures and hence found the image difference visualization to be particularly useful when styling these figures to pinpoint elements that still require updates.

7 Discussion

Below we summarize the limitations of our difference visualization for images and data visualizations, scalability limitations of the notebook's history and content, limitations during collaboration or in reactive notebooks, and future plans on controlling the provenance aggregation.

Image Differences. We opt for a detailed pixel-based approach (1) because the difference visualization is part of a broader context in the notebook diff, also highlighting changes to the underlying data or the generating code in the preceding cells; and (2) because it makes our approach independent of the programming language and library being used (e.g., seaborn [65] and Yellowbrick [5] in Sec. 5.2). But the pixel-based difference approach is sensitive to images of varying sizes or internal shifts: Fig. 6 encodes the title, grid lines, and x-axis as changed due to a slight shift to the left. Semantic comparison, aware of the data and how it is represented, would avoid such incorrect differences and could allow users to focus on specific differences in their comparison.For example, during our interviews, one user expressed interest in seeing differences in styling specifically (see Sec. 6). For other tasks, only how marks are affected by data changes may be relevant. ComputableViz [68] can compute differences between two visualizations, their data, or their style, but requires the visualization specifications and does not encode the differences. In the future, we would like to create extensions for Loops that provide difference visualizations for specific use cases or libraries. These could add semantic comparison , e.g., for seaborn, in addition to the current pixel-based approach. Currently we also do not consider interactivity in visualizations, which could be supported by adding Persist [18] as an extension.

Scalability. The compact notebook diff scales well with an increasing number of cells. However, the number of versions depends on the user's execution patterns, and horizontal space is limited. Visualizing code differences within the notebook diff also faces spatial constraints, often requiring users to scroll horizontally within the cell to view differences fully. Our attempts to reduce code differences to the neighborhood of changed content encountered challenges. Especially when exploring a cell's history, the individual changed code parts should remain comparable. To address this, we are considering a more nuanced degree-of-interest function to control the amount of visualized code in a changed version and its adjacent versions [2]. In the notebook diff, the pixel-based difference visualization for tabular data faces similar spatial constraints, as already discussed for TACO [44]. Due to the limited horizontal space, only a few hundred columns can be displayed without scrolling. However, we argue that our visualization scales significantly better than the output in the notebook itself (see Appendix). The detailed difference visualization of tabular data shown when comparing a cell also displays the table content and faces the same constraints as the table output in the notebook. The pandas library [60] truncates tables to 10 rows and 20 columns by default when output in the notebook. Our difference visualization relies on this output, showing only changes within it. This has led our users to express a desire to see a full diff (see Sec. 6). However, this would require implementations tailored to different programming languages and environments, which we believe is better realized by specific extensions.

Collaboration and Reactive Notebooks. Collaboration and coauthoring of notebooks are crucial aspects of data analysis [37]. The notebook users we interviewed rarely collaborate with colleagues on a notebook. And when they do, they take turns working with them on the notebook. Loops already effectively supports such asynchronous collaboration by visualizing contributors to notebook versions and cell changes. For real-time collaboration, the suitability of our approach to aggregate notebook provenance varies depending on the collaboration style. In a study by Wang et al. [62], half of the teams collaborating in real time split their tasks to explore alternate solutions. Editing and executing code in different parts of the notebook simultaneously can result in more notebook versions than the analysts intended.

Some scholars argue that reactivity is a prerequisite for real-time collaboration [47]. Reactive notebooks automatically update the output as the data used by these outputs change, removing concerns about out-of-order executions. We still see advantages in using Loops with reactive notebooks. First, modifying a single cell can immediately affect multiple outputs, and Loops helps users recognize and understand these changes. Second, tracking provenance remains important to understand the evolution of analysis or comparing alternatives. However, reactive notebooks do not have to follow the same structure as sequentially executed notebooks (see Sec. 3). Automatic re-evaluation of cells after a change can thus generate unintended versions of the notebook.

Provenance Tracking and Aggregation. In the future, our goal is to improve users' control over the provenance tracking and aggregation. We want to enable users to curate the notebook's provenance and to split or merge notebook states. Additionally, we want to offer further aggregation methods, based on contributor, time, or manual saves of the notebook, which users can combine to better support the scenarios described above.

8 Conclusion

Analysts face challenges and pain points when working with notebooks [10]. With the Loops approach described in this paper, we address the challenges related to tracking and comparing notebooks. Loops tracks the provenance of notebooks to assist analysts during their work. We visualize the evolution of the notebook over time and highlight differences between versions. We have carefully designed visualizations that consistently visualize changes for the whole notebook and various types of content present in notebooks. This gives analysts direct feedback on their changes and supports them at various stages of the data science process. Based on the feedback from four notebook users, we are confident that Loops can effectively support data science processes in notebooks.

Supplemental Materials

All supplemental materials are available on OSF at osf.io/79eyn. In particular, they include (1) a full version of this paper with all appendices, (2) a video to demonstrate the workflow and interactions in Loops, and (3) the source code of our prototype together with the datasets used for the uses cases and all figures of our presented approach.

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