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Automatic Module Detection in Data Cleaning Workflows: Enabling Transparency and Recipe Reuse

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Abstract

Before data from multiple sources can be analyzed, data cleaning workflows ("recipes") usually need to be employed to improve data quality. We identify a number of technical problems that make application of FAIR principles to data cleaning recipes challenging. We then demonstrate how *transparency* and *reusability* of recipes can be improved by analyzing dataflow dependencies within recipes. In particular column-level dependencies can be used to automatically detect independent subworkflows, which then can be reused individually as data cleaning modules. We have prototypically implemented this approach as part of an ongoing project to develop open-source companion tools for OpenRefine.

Keywords: Data Cleaning · Provenance · Workflow Analysis

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Introduction and Overview

The FAIR guiding principles for scientific data aim to ensure that data is *findable*, *accessible*, *interoperable*, and *reusable* (Wilkinson et al., 2016). Metadata in general and *provenance* information in particular can be used to improve reusability of data and the reproducibility of results by increasing *transparency* (Nosek et al., 2015; McPhillips et al., 2019). A major reason to provide provenance information is to increase the trustworthiness of data by laying open its *lineage*, i.e., its origins and processing history. It is also often pointed out that data analysis consists of at least 80% "wrangling and cleaning" of data, leaving only 20% for the data analysis proper. Not surprisingly, data cleaning "recipes" (or *workflows*) are of central importance in data analysis and should thus follow principles similar to FAIR data; in particular they should be *transparent* and *reusable*.

Consider a user U (a researcher or data curator) who wants to prepare a dataset D_0 for analysis as part of a scientific study. Upon inspection she quickly realizes that D_0 is not "fit for purpose" (Chapman et al., 2020), i.e., its organization and data quality needs to be improved for the intended use cases. She then employs a data cleaning tool such as OpenRefine (OR, 2021) to obtain a "cleaner" version that can be used for the subsequent analyses.

An important byproduct of U's interactive data cleaning process is an *operation history* H that can be used to describe her data cleaning workflow as a sequence of *steps* $S_1, \ldots, S_n$ that transform the given D_0 via intermediate snapshots into a final version D_n:

$$D_0 \overset{S_1}{\rightsquigarrow} D_1 \overset{S_2}{\rightsquigarrow} D_2 \overset{S_3}{\rightsquigarrow} \cdots \overset{S_n}{\rightsquigarrow} D_n \ . \qquad (H)$$

This operation history H can be understood as a form of *provenance* information that increases the transparency of the data cleaning process. It contains *prospective* elements at the *workflow level*, e.g., the names of operations used, and *retrospective* provenance at the *trace level*, e.g., the concrete value changes and parameter settings used in each step.

Technical Challenges and Approach

The first practical challenge is how to present the history H in a form that helps users (the original workflow creator U, possible auditors, and other potential users) *understand* the data cleaning workflow, both at a higher, conceptual level, and at a more detailed level. We call this the **transparency problem** for H.

A second challenge for U is how to identify and extract from H one or more *reusable recipes* $R \subseteq H$, i.e., those elements and subworkflows of the data cleaning history that can be reused for other datasets. We call this the recipe **reusability problem**.

There are a several other technical challenges worth mentioning: While U is exploring and cleaning a dataset, she occasionally has to backtrack and undo earlier steps to modify her workflow. To this end, OpenRefine provides an *undo/redo* operation stack to support the back-and-forth of this interactive process. She can backtrack from the current step S_k to an earlier step S_i, inspect the dataset at that point, and then redo the steps $S_{i+1}, \ldots, S_k$. Once she decides to modify S_i, however, the subsequent steps $S_{i+1}, \ldots, S_k$ are typically discarded.[1] If a user wants to retain some or all of these steps, they can try to work around

[1] The rationale is that a change in S_i may invalidate the subsequent steps $S_{i+1}, \ldots, S_k$.

the limitations of the tool, e.g., by saving the steps to be re-executed and then trying to reapply them after the modified step S_i. The **history update problem** is to determine which of the steps $S_{i+1}, \ldots, S_k$ need to be discarded because they no longer apply, or how to modify them so they remain applicable.

Recipe migration problem. When presented with a new but similar dataset D'_0, a curator U may want to reuse the parts of the history H that seem applicable not just to D_0, but more generally to other datasets similar to it (such as D'_0). Thus U wants to select a recipe $R \subseteq H$ for reuse, possibly revising it as needed. Indeed R is often not applicable to D'_0 directly, but may have to be modified further to account for the *schema differences* between D_0 and D'_0.

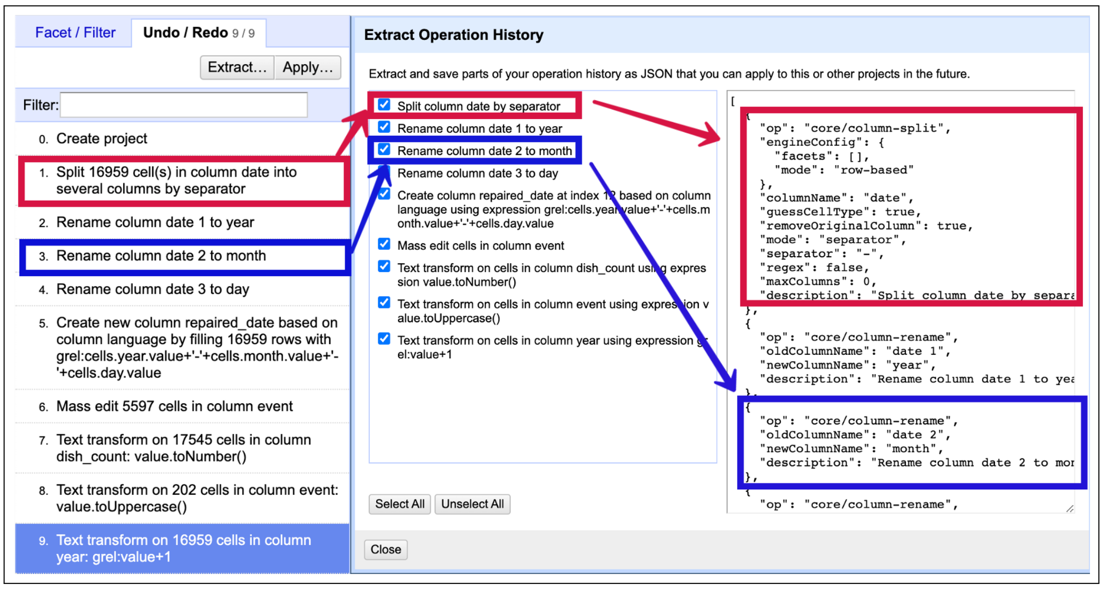
Recipe evolution problem. Finally, a user may want to share a recipe with a wider audience, in the spirit of the FAIR principles. To this end, she plans to subject each candidate recipe R_0 to a number of tests before publishing it. Lessons learned from the tests result in a sequence $R_0 \rightsquigarrow R_1 \rightsquigarrow \cdots \rightsquigarrow R_\ell$ of modifications to and variants of the original recipe. The problem is how to support this evolution from R_0 to a publishable recipe R_ℓ, i.e., how to effectively modify, organize, and test recipes.

Contributions. In this paper, we focus on solving the *transparency problem* and one aspect of the *reusability problem*. We employ an underlying provenance model for data cleaning that can be used to describe data dependencies at different levels of granularity: e.g., in a **table view**, we view a history H as a sequence of snapshots $D_0, D_1, \ldots, D_n$ in which each new snapshot D_{i+1} is derived from its predecessor D_i via a transformation step S_{i+1}. In this way, using a coarse-grained table view, a user can get a first, high-level overview about a data cleaning workflow. On the other hand, a finer-grained dependency analysis will take into account the *columns* that an operation reads and writes, using the input-output *signatures* of the data transformation functions that implement a step S_i in the workflow. The resulting **schema view** paints a more detailed and transparent picture of how the workflow operations act on the schema, as the dataset is being transformed, step by step. Finally, the **modular view** provides another column-oriented view on the workflow: Similar to the schema view, column-level dependencies are obtained from the recipe's dataflow graph, but now *independent subworkflows are automatically identified*, which can then form the basic building blocks (or *modules*) of reusable recipes.

Both the schema view and the modular view rely on a *classification of operations* in order to highlight the different kinds of effects that workflow steps have on a dataset and its schema: many transformations operate on a single column, while others read or write multiple columns or rename columns; some operations are *generic* (i.e., can be applied, in principle, on any dataset column, e.g., `toLower` or `toUpper`), while others are *domain-specific* and *user-defined* (e.g., a custom mapping that fixes common misspellings over a controlled vocabulary of city names); yet other operations convert data types (e.g., from string to number), etc. We have prototypically implemented our approach as part of an ongoing project to develop open-source companion tools for OpenRefine (Li, 2021).

Data Cleaning Workflows and OpenRefine

OpenRefine is a popular open-source data cleaning tool that allows users to execute data transformations in a browser-based, spreadsheet-like UI (OR, 2021). As shown in Figure 1, the tool allows users to export an operation history H as a recipe R by selecting



0. Create project
1. Split 16959 cell(s) in column date into several columns by separator
2. Rename column date 1 to year
3. Rename column date 2 to month
4. Rename column date 3 to day
5. Create new column repaired_date based on column language by filling 16959 rows with grel:cells.year.value+'-'+cells.month.value+'-'+cells.day.value
6. Mass edit 5597 cells in column event
7. Text transform on 17545 cells in column dish_count: value.toNumber()
8. Text transform on 202 cells in column event: value.toUppercase()
9. Text transform on 16959 cells in column year: grel:value+1

Extract Operation History

Extract and save parts of your operation history as JSON that you can apply to this or other projects in the future.

- [✓] Split column date by separator
- [✓] Rename column date 1 to year
- [✓] Rename column date 2 to month
- [✓] Rename column date 3 to day
- [✓] Create column repaired_date at index 12 based on column language using expression grel:cells.year.value+'-'+cells.month.value+'-'+cells.day.value
- [✓] Mass edit cells in column event
- [✓] Text transform on cells in column dish_count using expression value.toNumber()
- [✓] Text transform on cells in column event using expression value.toUppercase()
- [✓] Text transform on cells in column year using expression grel:value+1

```
[
  {
    "op": "core/column-split",
    "engineConfig": {
      "facets": [],
      "mode": "row-based"
    },
    "columnName": "date",
    "guessCellType": true,
    "removeOriginalColumn": true,
    "mode": "separator",
    "separator": "-",
    "regex": false,
    "maxColumns": 0,
    "description": "Split column date by separa
  },
  {
    "op": "core/column-rename",
    "oldColumnName": "date 1",
    "newColumnName": "year",
    "description": "Rename column date 1 to yea
  },
  {
    "op": "core/column-rename",
    "oldColumnName": "date 2",
    "newColumnName": "month",
    "description": "Rename column date 2 to mor
  },
  {
    "op": "core/column-rename",
```

Figure 1. OpenRefine History and Recipe. The undo/redo history H (*left*) shows the steps previously executed. After clicking "Extract", the user can select the operations to be exported via a checklist (*middle*). The selected recipe operations $R \subseteq H$ then appear in the JSON panel (*right*). Steps 1 (column-split) and 3 (column-rename) are highlighted in the history, the checklist, and the JSON recipe. Example taken from a recipe for the *menus dataset*, crowd-sourced by volunteers for the New York Public Library (New York Public Library, 0 01).

a set of operations $R \subseteq H$. The resulting recipe can be copied and later reused for other datasets.

On the left of Figure 2, a typical data cleaning use case is depicted: the user employs OpenRefine to clean a dataset D_0. The process $D_0 \overset{H}{\rightsquigarrow} D_n$ generates an operation history H with n steps $S_1, \ldots, S_n$ from which the user can select a recipe $R \subseteq H$ (see Fig. 1). This recipe can then be exported in an OpenRefine-specific JSON format for later reuse. Since R is not meant for "human consumption", it is rather opaque and hard to digest for users.

A first step towards improving transparency is to create a *workflow model* from R. We previously developed or2yw[2], which automatically generates YW annotations from R. The YW tool uses these to create a workflow model that can be queried and visualized (McPhillips et al., 2015). YW was originally developed to allow researchers a simple way to manually annotate their program scripts in order to reveal workflow steps and dataflow dependencies implicit in those scripts, thereby turning an opaque script into a transparent workflow. With the help of or2yw the user can *automatically* generate YW models from OpenRefine recipes (rather than manually creating them), thus providing a more transparent workflow view on a previously executed sequence of data cleaning operations. For a given workflow model, the YW tool can generate several different views, e.g., a *combined view* which depicts a workflow as a directed graph, linking steps via the data that flows between them; a *process view* that emphasizes steps; and a *data view* that highlights data derivations.

We have since implemented ORMA (**O**pen**R**efine **M**odel **A**nalysis), a new OpenRefine

[2] or2yw: an **O**pen**R**efine-*to*-**Y**es**W**orkflow mapping tool (Li et al., 2021).

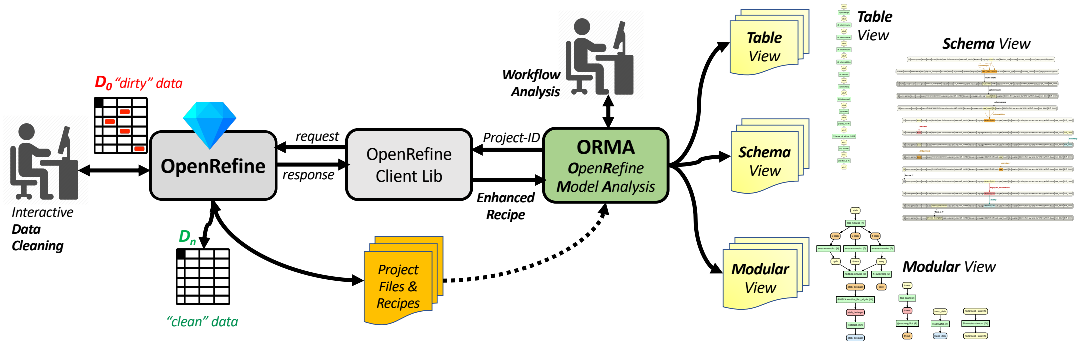


Figure 2. A user cleans dataset D_0 with OpenRefine, obtaining an improved version D_n, along with internal project files and recipes. During workflow analysis, the user provides ORMA with a project-ID, which is then used to generate an enriched recipe (i.e., a workflow model). The tool then analyzes data dependencies to generate multiple views: a high-level, linear *table view* closely corresponding to the sequential recipe, a *schema view* showing how columns are used and updated by each step; and a *modular view*, automatically restructuring the recipe into its independent subworkflows (*modules*).

companion tool that uses additional details about H from *project files* created by OpenRefine when a data cleaning project is saved. The ORMA prototype can then create "enriched" recipes from this information which in turn are used to create new knowledge products (*table view*, *schema view*, and *modular view*) as illustrated in Figure 2.

Modeling Data Cleaning Workflows

Before taking a closer look at some of the new views and visualizations that ORMA supports, let us first consider the underlying workflow, provenance, and data models.

Modeling Workflows and Provenance

On the left of Figure 3, two modeling levels for data cleaning recipes are depicted:

- At the upper **workflow level** an operation such as "$Y = F(X)$" stands for any data transformation that reads some data X (e.g., from a table, a column, or a cell) and that produces some output data Y.[3]
- At the lower **trace level**, a concrete value $x_i \in X$ is *used* by an invocation "$y_i = F_i(x_i)$" to *generate* a result value $y_i \in Y$.

The data cleaning recipes of OpenRefine can thus be understood as workflow-level, *prospective* provenance, since they prescribe what operations should be executed (and in which order) when the recipe is to be reused. But since recipes R are obtained from operation histories H, they also constitute *retrospective* provenance information, since at least a partial record of the processing history is recorded by them.

In addition, OpenRefine captures more detailed retrospective provenance in its internal *project files* (cf. Figure 2), e.g., *parameter values* used at runtime by certain operations, and *deltas* that can be used to recreate any intermediate snapshot D_i when the user employs the undo/redo feature of OpenRefine.

[3] Note that this includes the special case that Y represents the updated version of X.

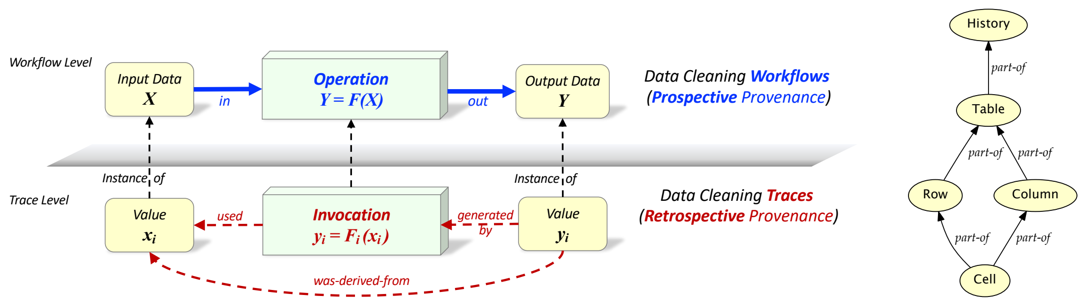


Figure 3. Workflows, Traces, and Data Granularity. A data cleaning recipe (*workflow*) consists of data transformations (*operations*) of the form "$Y = F(X)$", i.e., where a function is applied to an input X to obtain output Y (*upper left*). Workflows are a form of *prospective provenance*. At runtime, an *invocation* "$y_i = F_i(x_i)$" yields *retrospective provenance*, e.g., describing that y_i *was generated by* F_i, which in turn *used* x_i (*lower left*). The data being processed can be modeled at different *levels of granularity* (*right*): a cell can be identified by the row and column it is part of; tables consist of rows and columns, and can have a history (implying that rows, columns, and cells also have a history).

On the right of Figure 3, a simplified version of the underlying **data model** is depicted. It shows that individual *cells* are part of *rows* and *columns*, which in turn are part of a data *table* D_i. Each table is part of a table *history*, i.e., a sequence of snapshots $D_0, \ldots, D_n$. The power of ORMA and similar tools derives from the use of a flexible underlying model that combines prospective and retrospective information to describe data cleaning workflows, while simultaneously supporting different data granularities (e.g., *table*, *column*, *cell*) when describing relationships between elements. This combination allows one to create many types of relationships between the modeling elements, beyond the simple binary relationships (*in*, *out*, *used*, *generated-by*, and *was-derived-from*) depicted in Fig. 3.

Modeling Data Transformations

The final ingredient needed by ORMA to analyze data cleaning recipes as workflows is information about data transformations (operations): for each data cleaning operation or function F, we need to know at least its *signature* $F : \bar{X} \longrightarrow \bar{Y}$, i.e., the column(s) $\bar{X} = X_1, \ldots, X_k$ that F reads (or *uses*) and the column(s) $\bar{Y} = Y_1, \ldots, Y_m$ that it writes (or *generates*). In this way, by analyzing direct and indirect dependencies between operations of a workflow, we can create different workflow views, including a modular view which automatically detects independent subworkflows.

Consider two consecutive steps S_i and S_{i+1} in a workflow. A fundamental question is to determine whether S_{i+1} depends on S_i (so execution must be serial) or whether S_{i+1} is in fact *independent* of S_i (which can be modeled using a parallel branch in the workflow).

If the two steps are implemented by two operations $F_i : \bar{X}_i \longrightarrow \bar{Y}_i$ and $F_{i+1} : \bar{X}_{i+1} \longrightarrow \bar{Y}_{i+1}$, we can test whether $\bar{Y}_i \cap \bar{X}_{i+1} = \emptyset$. If this is the case, then the input $\bar{X}_{i+1}$ of S_{i+1} does not make use of any output $\bar{Y}_i$ of S_i, and we can say that S_{i+1} is independent of S_i. In this way, a data cleaning recipe can be modeled as a workflow graph consisting of *data nodes* that represent schemas or columns, and *transformation nodes* that represent the steps (data cleaning operations) of the workflow.

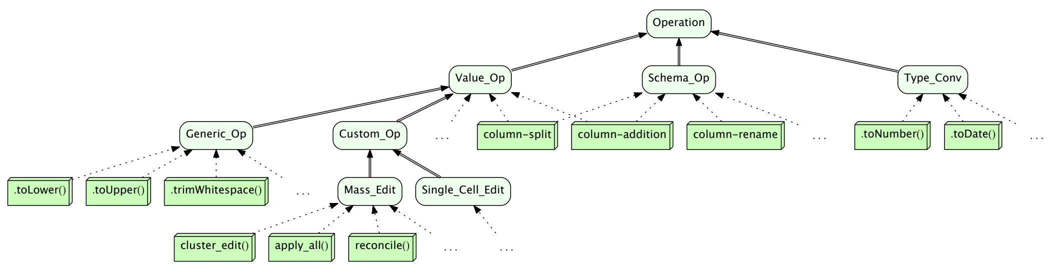


Figure 4. Classifying Operations: OpenRefine implements a range of data transformations, from simple, generic operations (toLower(), toUpper(), . . .) to powerful domain-specific operations requiring user interaction (e.g., for *clustering*, *normalizing*, and *reconciling* values), all the way to user-defined operations (e.g., using *regular expressions*).

Classifying Data Transformations

To make graphical workflow views more informative and intuitive for the user, different shapes and colors can be used in ORMA. For example a *table view* (as in Fig. 5 on the left) is depicted as a bipartite graph in which rounded yellow boxes represent table snapshots D_i, and green boxes represent workflow steps S_i that transform one snapshot to another. For more detailed views such as the *schema view* and the *modular view*, it is helpful to classify operations according to their shared properties, and then use colors (and/or shapes) to highlight the different effects that related operations have on the data tables.

Figure 4 depicts a (very incomplete) view of a possible classification of the built-in operations in OpenRefine: many operations change data values (Value_Op), some change the data schema (Schema_Op), and yet others the data type (Type_Conv). Often it is also useful to distinguish generic operations (Generic_Op) from domain-specific operations (Custom_Op). While the former can be applied, in principle, on any data column, the latter may be applicable only for certain domains of data (e.g., a mapping from common variants and mispellings of city names to their canonical representation). There are many other ways to organize and classify operations, depending on the desired perspective or use of the classification. In the current version of the ORMA tool, custom operations (such as single cell edits and certain mass edits) are prominently highlighted in red, while generic operations are highlighted in orange (cf. Figure 5 and Figure 6).

Transparency and Recipe Reuse through Workflow Views

We are now ready to describe how ORMA, our **O**pen**R**efine **M**odel **A**nalysis tool, can be used to increase the transparency of data cleaning recipes and facilitate their reuse.

ORMA Table View

When using OpenRefine to clean a dataset, an operation history H is created, allowing the user to extract some of the operations as a recipe $R \subseteq H$ (Figure 1). Additional provenance details can be obtained from internal project files (Figure 2) which ORMA can then use to create different workflow views. The **table view** on the far left in Figure 5 depicts a linear workflow that corresponds one-to-one to an operation history (similar to the one in

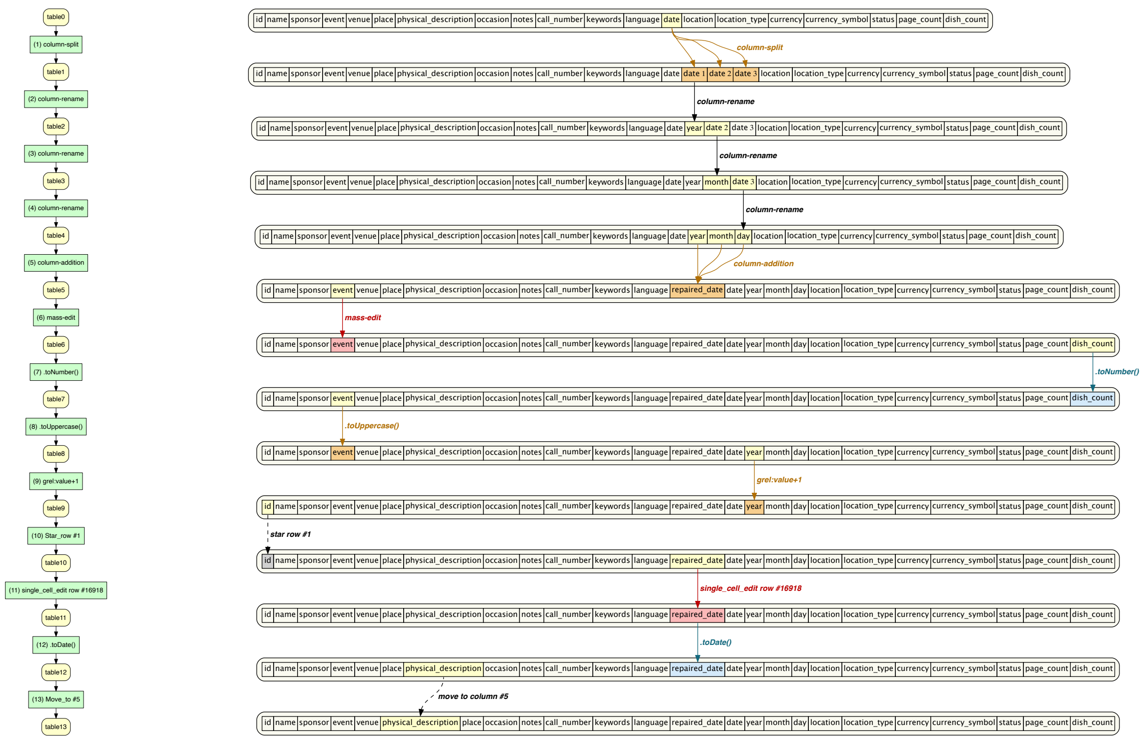


Figure 5. Table View vs Schema View. In the **table view** (*left*) individual columns are not shown, and every snapshot table_{i+1} depends on its immediate predecessor table_i. In the **schema view** (*center, right*) a summary of changes to the schema and column-level operations is depicted: The user first worked on several date columns, then the event column (and other columns) before returning again to some specific edits on the repaired_date column. Columns are colored according to the type of operation that affected the column.

Fig. 1), thus making it easy for a user to see the correspondence between the two. Through parameter switches, ORMA can create different levels of detail for table views, e.g., for a high-level overview, operation parameters can be suppressed (as in Fig. 5) or alternatively, detailed parameter views can be added to table views.

ORMA Schema View

The **schema view** in Figure 5 is arguably more transparent than the table view: it stills shows the sequential (linear) nature of the table view, but it also reveals which columns are read and rewritten (updated or created anew) by each transformation step. Arrows are used to indicate column-level dependencies between steps; arrow labels indicate the names of operations; and colors are used to highlight the different nature of operations: columns updated through custom operations are shown in red (possibly requiring the most attention), generic operations in orange, and type conversions in (light) blue. Dashed arrows indicate user interactions in the OpenRefine UI, e.g., when a user "stars" (flags) rows, or when she is reordering columns (e.g., physical_description: move to column #5).

The schema view in Figure 5 also provides additional insights, e.g., it reveals that the data curator was "jumping around" between different columns when cleaning the original dataset: while the first operations (near the top and middle of the evolving schema) operate on the date column and its derivative columns, two subsequent changes are then executed on the event column (with an additional "interruption" by an operation on dish_count). Only near the end of the workflow does attention return to the repaired_date column that had been created in earlier steps.

ORMA Modular View

Figure 6 again shows a table view on the far left (for orientation and comparison) and an automatically created **modular view** in the center, right. Upon close inspection of the schema view in Figure 5, one can already guess at least some elements of the subworkflow structure exposed by the modular view. As in the schema view, the modular view depicted in Figure 6 uses different colors to indicate the nature or type of the operations involved (e.g., generic, custom, type conversion). ORMA automatically detects all independent subworkflows (*modules*) based on the column-level dependencies obtained from recipes and the function signatures of operations. The modular view shown in Figure 6 still contains the original sequence numbers of workflow steps, which helps in matching steps across alternative views of the same workflow. In particular, the coarser-grained linear table view could be constructed from the modular view (but not vice versa). Modular subworkflows as the ones shown here can be used as reusable building blocks for composing larger data cleaning recipes from a library of independent modules. Different levels of transparency and "verbosity" can be chosen for the different views supported by ORMA: e.g., detailed parameter values can be included in the views, along with other derived information (e.g., how many canonical names are part of a mass-edit and how many variant spellings are recognized for each canonical name). We have omitted the display of these additional details in our figure here.

Conclusions

We have presented an approach to improve the transparency and reusability of data cleaning recipes. The key idea is to model recipes as workflows over a suitable data model for describing data cleaning processes. We have prototypically implemented an OpenRefine model analyzer tool, ORMA (Li, 2021) which can be used to create different types of workflow views, from simple linear table views, via informative schema views, to modular views that automatically identify independent subworkflows that facilitate reuse. In future work, we plan to tackle several other technical challenges mentioned earlier, e.g., the history update problem or the recipe migration problem. Another direction for future work includes the use of retrospective provenance information to obtain even more powerful analysis methods based on hybrid models of provenance.

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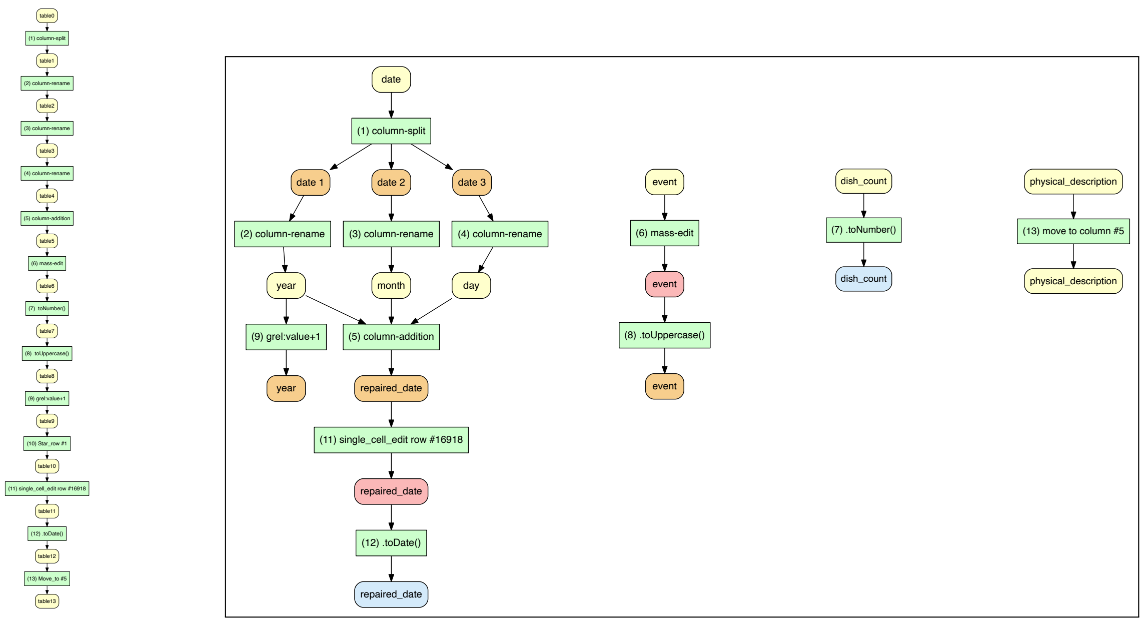

Figure 6. Table View vs Modular View. The table view on the left suggests (correctly) that each table snapshot depends on its predecessor via a workflow step. On the other hand, the **modular view** on the right highlights that the linear workflow can be decomposed into four *independent* subworkflows (*modules*), based on a finer-grained *column-level* dependency analysis: The largest module starts from the date column, expands it by creating (and renaming) separate columns for year, month, and day, eventually yielding a repaired_date column. The other three modules are single-column subworkflows, each working on their own column (event, dish_count, and physical_description).

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