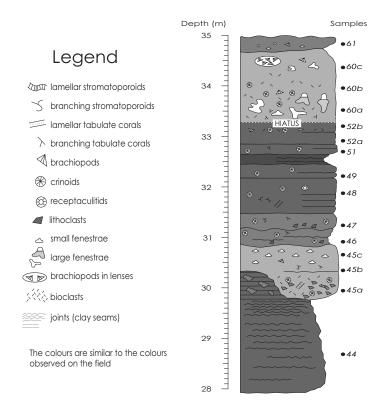
# StratigrapheR: Concepts for Litholog Generation in R

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**Abstract** The **StratigrapheR** package proposes new concepts for the generation of lithological logs, or lithologs, in R. The generation of lithologs in a scripting environment opens new opportunities for the processing and analysis of stratified geological data. Among the new concepts presented: new plotting and data processing methodologies, new general R functions, and computer-oriented data conventions are provided. The package structure allows for these new concepts to be further improved, which can be done independently by any R user. The current limitations of the package are highlighted, along with the limitations in R for geological data processing, to help identify the best paths for improvements.

#### 1 Introduction

**StratigrapheR** is a package implemented in the open-source programming environment R. **StratigrapheR** endeavors to explore new concepts to process stratified geological data. These concepts are provided to answer a major difficulty posed by such data; namely a large amount of field observations of varied nature, sometimes localized and small-scale, can carry information on large-scale processes. Visualizing the relevant observations all at once is therefore difficult. The usual answer to this problem in successions of stratified rocks is to report observations in a schematic form: the lithological log, or litholog (e.g., Fig. 1). The litholog is an essential tool in sedimentology and stratigraphy and proves to be equally invaluable in other fields such as volcanology, igneous petrology, or paleontology. Ideally, any data contained in a litholog should be available in a reproducible form. Therefore, the challenge at hand is what we would call "from art to useful data"; how can we best extract and/or process the information contained in a litholog, designed to be as visually informative as possible (see again Fig. 1).



**Figure 1:** Example of a computer-drawn litholog of calcareous rocks, modified from Humblet and Boulvain (2000) using vector graphics software (e.g., Inkscape, CorelDRAW, or Adobe Illustrator).

Lithologs can be hand-drawn, computer-drawn, or generated via ad hoc software tools. Drawn figures can have unlimited precision and personalization. They are, however, time-consuming to produce and ill-adapted for the extraction of data for further numerical analysis. Moreover, any modification to drawn lithologs has to be performed manually. Ad hoc software tools such as the open-source SedLog program (Zervas et al., 2009) or the SDAR R package (Ortiz et al., 2019) propose a solution to such short-comings by generating lithologs from geological data provided in a text format. The most common text format is the American Standard Code for Information Interchange -ASCII-ASCII is used for the SedLog data format and for the Log ASCII Standard -LAS- (Heslop et al., 1999). The latter (LAS) is the data format used by the SDAR package.

A major advantage of ad hoc software tools is that any change in the data can automatically lead to an update in the display of the litholog. However, ad hoc software tools only permit a certain amount of personalization. The graphical output of ad hoc software tools, which can be obtained in vector graphics format (e.g., in the Scalable Vector Graphics [SVG] format), has to be post-processed in vector graphics software to add elements that are not supported by the data format. In SedLog, for instance, to add plots next to the litholog (i.e., to visualize quantified analytical values and their relation to the lithological features) the plots need to be generated separately and then added manually along the litholog in vector graphics software. SedLog does permit a certain amount of personalization, but only for the lithological symbology, by giving the user the option of adding self-made symbology (e.g., to show the position of paleontological or sedimentological features). In the SDAR package, the only data automatically displayable are Gamma Ray spectrometry values, and the symbology (for lithology, fossils, etc.) cannot be personalized.

Generally speaking, the graphical style of the lithologs generated by ad hoc software tools is difficult to personalize entirely. To do so, each functionality has to be modular, which is better done in a scripting language such as R. Yet, the **SDAR** package, although coded in R, is not modular. All the plotting is made using a single function. Any personalization feature would need to be explicitly coded into that function, which would be a never-ending task. Moreover, ad hoc software tools are difficult to update and improve. Adding new functionalities or maintaining the software for compatibility with new operating systems, for example, usually falls on the shoulders of the developers of that software.

The **StratigrapheR** package is presented here as a new mean to generate lithologs. It provides a complementary approach to the existing methodologies and circumvents the aforementioned problems. **StratigrapheR** is designed not around a specific data format but on general tools able to deal with different formats. This opens a way of processing the geological data through a scripting language which has a large potential to evolve. **StratigrapheR** shows that symbiosis between automation and personalization is achievable for litholog generation. As it stands, the package does not meet the "from art to useful data" challenge entirely. However, it is a proof of concept showing that, despite the artistic nature of lithologs, they can be based on usable digital data, or that conversely, usable data can be extracted from drawn lithologs.

**StratigrapheR** is coded in R, which disposes of automated package checks (Wickham, 2015) and is itself updated regularly. This is one mechanism against the inevitable obsolescence of the functionalities. Similarly, as the **StratigrapheR** package is structured in distinct basic functions, implementing new functionalities (or updating existing ones) can be done more easily by any user. Furthermore, the processing of geological data, whether to generate lithologs or for any other procedure (among others plotting proxies, applying moving averages on these proxies, or performing spectral analysis), can directly be performed in R (see, for instance, the **paleotree** package for paleontology (Bapst, 2012), the **IsoplotR** package for geochronology (Vermeesch, 2018), or the **hht** (Bowman and Lees, 2013), **astrochron** (Meyers, 2014), **biwavelet** (Gouhier et al., 2019) and **DecomposeR** (Wouters, 2020) packages for spectral analysis). This means that the entire data treatment and visualization could be performed in a single scripting environment: R.

The main concepts for the use of **StratigrapheR** are presented in this paper. The current limitations of **StratigrapheR** and R for the processing of geological data are also highlighted to give an idea of the obstacles that the future developers will need to overcome to make R a better tool for geological data processing. Throughout the paper, examples are provided on how to make lithologs and how to process geological data. They can be run in R (you can download R here); the current version of **StratigrapheR** (1.2.3) works only on R 4.0 or higher versions. A GitHub repository is available at <a href="https://github.com/sewouter/StratigrapheR">https://github.com/sewouter/StratigrapheR</a>, where outside users can suggest improvements and provide feedback. The free RStudio interface is advised to use **StratigrapheR** in the R environment. The **StratigrapheR** package can be installed by typing:

install.packages("StratigrapheR")

To be used, the **StratigrapheR** package has to be loaded each time R or RStudio are opened, via the following code:

library(StratigrapheR)

#### 2 Data importation and processing

Data of any form can easily be imported using basic R functions, such as read.table() or readLines() for text files. Excel files can be downloaded using, for instance, the read.xlsx() function from the xlsx package (Dragulescu and Arendt, 2020). We advise putting any tabular data into data frame form (i.e., a table), which can be done via the data.frame() function.

As stratigraphic data can be found in an interval form (e.g., a specific strata between 25 and 30 m in a record, or the Jurassic between ca. 200 and ca. 145 million years ago), a formal scheme to deal with such data is provided: the 'lim' object (named after the xlim and ylim parameters that define the boundaries of plots in common R graphical functions) and a suite of functions that are associated to lim objects. The idea is to set a logical data format for intervals and to be able to manipulate these intervals in R. The lim objects are made via the as.lim() function by providing boundaries in the form of the 1 and r arguments, which respectively stand for left and right boundaries. The actual order of the boundaries is irrelevant to avoid unnecessary data cleaning (which is the reason why 'left' and 'right' were chosen as a convention rather than 'up' and 'down'). Each interval can be identified using the id argument. Providing the upper and lower boundaries allows taking gaps into account in lithologs, contrary to simply providing the thickness of layers (also called beds). Whether the boundaries are included in the interval can be determined via the b argument, which defines the boundary rules. This is an abstract feature, especially for geology purposes, because it is usually of negligible importance whether the infinitesimal position of a boundary is included in a given interval. However, taking this into account is critical to explicitly describe the behavior of intervals. This can be used, for instance, to assign an interval to a sample located at the common boundary between two intervals that do not overlap otherwise. By providing a boundary rule, it can be explicitly assigned to only one of the two intervals, none of them, or both of them. The boundary rule is expressed by characters, and can be set to "[]" (or "closed") to include both boundary points, "][" (or "()", and "open") to exclude both boundary points, "[[" (or "[)", "right-open" and "left-closed") to include only the left boundary point, and "]]" (or "(]", "left-open", and "right-closed") to include only the right boundary point. The left element (e.g., the [ of "[]") stands for the left boundary (not necessarily the lowest one), while the right element (e.g., the ] of "[]") stands for the right boundary (not necessarily the highest one). We illustrate how to visualize intervals with the following code (note: graphics generated by code in the article are shown directly after the code that generates them):

```
interval \leftarrow as.lim(1 = c(0,1,2), r = c(0.5,2,2.5),
                                                       # Make a lim object
                    id = c("Int. 1","Int.2","Int.3"))
interval # print what is in the lim object
#> $1
#> [1] 0 1 2
#> $r
#> [1] 0.5 2.0 2.5
#> $id
#> [1] "Int. 1" "Int.2" "Int.3"
#> [1] "[]" "[]" "[]"
# Visualization of the lim object
plot.new()
plot.window(ylim = c(-0.5, 2.5), xlim = c(0, 2.5))
axis(3, pos = 1.5, las = 1)
infobar(ymin = 0, ymax = 1, xmin = interval$1, xmax = interval$r,
        labels = c(interval$id), srt = 0)
                                                                 2.5
                       0.0
                               0.5
                                        1.0
                                                1.5
                                                         2.0
                          Int. 1
                                                Int.2
                                                             Int.3
```

Functions are provided to characterize the relationships of intervals with each other: are.lim.nonunique() checks whether the intervals are of non-zero thickness (e.g., unlike [1,1]), are.lim.nonadjacent() checks if the intervals do not share any adjacent boundaries, and are.lim.distinct() checks whether the intervals are not overlapping. The simp.lim() function is provided to merge adjacent and/or overlapping intervals having identical IDs. The flip.lim() function is provided to find the complementary intervals of a set of intervals (i.e., the gaps). The mid.lim() function provides a way to define intervals in between data points. If all different intervals are strictly non-overlapping for all values (for instance, the intervals [0,20[ and [20, 100] are non-overlapping and therefore 20 is uniquely represented by the second interval), the in.lim() function can be used to find which values belong to which respective intervals. Typically, such functions can be used to craft stratigraphic intervals (such as magnetochrons or stages) and determine the beds or samples that are in or outside them.

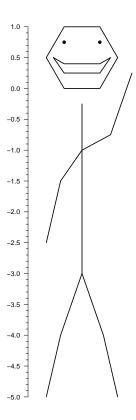
## 3 General plotting considerations

The first challenge when plotting a litholog is its size: a litholog needs to be detailed at a small scale (typically at the centimeter scale for high precision) while spanning the entirety of a record (up to hundreds of meters). This makes lithologs sometimes quite extended. This is problematic considering that the classical R graphic window is not adapted to visualize anything exceeding the size of the computer screen. To remedy this problem, the pdfDisplay() function is here introduced, which draws plots directly in a PDF (Portable Document File) document and opens it in the computer's default PDF reader. This PDF document can have any size desired by the user, and therefore, allows visualizing all the details of a very long litholog. This is illustrated by the code here below, which draws a vertically standing stickman. Depending on the screen, this vertical stickman could be difficult to visualize without pdfDisplay().

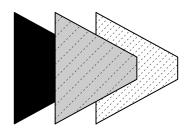
To avoid having to close the PDF reader at each change of the plot (as most PDF readers do not permit changes to the PDF file while it is displayed), each new PDF can be named differently: each new document version will have its name be followed by '\_(i)', where i is the version number (e.g., test\_(1).pdf, test\_(2).pdf, etc.). This practice is here referred as *tracking* the version number. It is noteworthy to cite the free Sumatra PDF software, which is available for Windows operating systems, and lets PDF files be modified while still displaying them without the trick of having to change the file name. In that case, the tracking of the version numbers can be canceled by setting the track parameter to FALSE. PDF files generated by pdfDisplay() can easily be imported into vector graphics software. The pdfDisplay() function also allows for the direct generation of an SVG file. pdfDisplay() is a wrapper of the more basic pdf() function (i.e., its code is based on the pdf() function); other PDF generating functions could be used interchangeably.

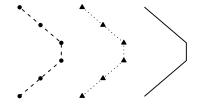
To make plots starting from an empty background, we advise using the plot.new() and plot.window() functions, which are of lower level (i.e., more basic) than the plot() function. They are used to create a completely empty plotting environment in which to add the litholog. To add axes, the axis() function is a versatile tool, which can be replaced by the minorAxis() function provided in **StratigrapheR** to add minor axis ticks. The minorAxis() function is itself a wrapper of the axis() function.

```
graphical_function <- function() # Graphical function needed by pdfDisplay
   opar <- par()$mar # Save initial graphical parameters</pre>
  par(mar = c(0,3,0,1)) # Change the margins of the plot
  plot.new() # Open a new plot
  plot.window(xlim = c(-0.2, 1.2), ylim = c(-5, 1)) # Define plot coordinates
  minorAxis(2, at.maj = seq(-5, 1, 0.5), n = 5, las = 1) # Add axis
  points(c(0.25, 0.75), c(0.75, 0.75), pch = 19)
   polygon(c(0.1, 0.25, 0.75, 0.9, 0.75, 0.25, NA,
             0, 0.25, 0.75, 1, 0.75, 0.25),
           c(0.5, 0.25, 0.25, 0.5, 0.4, 0.4, NA,
             0.5, 0, 0, 0.5, 1, 1), 1wd = 2)
  lines(x = c(0.5, 0.5, NA, 0, 0.2, 0.5, 0.8, 1, NA,
               0, 0.2, 0.5, 0.9, 1.2),
         y = c(-0.25, -3, NA, -5, -4, -3, -4, -5, NA,
               -2.5, -1.5, -1, -0.75, 0.25), 1wd = 2)
   par(mar = opar) # Restore initial graphical parameters
}
pdfDisplay(graphical_function(), "graphical_function", width = 3.5, height = 10)
```

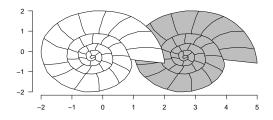


Adding every element of the lithologs symbology uses a very basic data format for polylines and polygons, which are respectively drawn using the multigons() and multilines() functions. These novel functions allow precise control of graphical parameters when drawing multiple polygons and polylines. These functions require an identification argument i, similar for each point of a single polygon or polyline, and the x and y coordinates of each point. The following code shows the use of the multigons() and multilines() functions:





The pointsvg() function is provided in **StratigrapheR** to import groups of polygons and polylines drawn in vector graphics software, under specific conditions: firstly, the drawing needs to be in SVG format; secondly, the pointsvg() function is only able to identify objects of class "line", "rect", "polygon", and "polyline" in the SVG file. The reason for this is that only these types of objects are simple lines, and polygons made of nodes linked together by straight lines. This means that pointsvg() is not able to recognize all the objects present in an SVG file. Furthermore, pointsvg() only identifies the coordinates of each objects, regroups them into separate polygons and polyline objects, and in which order to plot them. All other graphical parameters, such as color or line thickness, are not taken into account. These parameters have to be specified in the drawing functions. Objects obtained using pointsvg() on SVG files can be added using the framesvg() or centresvg() functions, which respectively add the object within a given frame or center the object on a given point.



It should be noted that repetitions of the same SVG object can be generated by a single call of the framesvg() or centersvg() functions. This facilitates the automation of the litholog generation. Modifications of the SVG objects can also be accomplished using the changesvg() function, which enables, among other things, to change the order of plotting of the polylines and polygons, remove some of them, or invert the figure in x and/or y. The framesvg() or centersvg() can also output the drawing with modified coordinates, which can be plotted using placesvg() (see, for instance, the code of the last example).

## 4 Generating lithologs

The data to make lithologs can be provided in the form shown in Table 1.

id	1	r	h	colour	litho
B1	0	1	3	grey	S
B2	1	3	4	grey	L
В3	3	4	5	black	C
B4	4	9	4	white	L
B5	9	11	4	white	L
					•••

**Table 1:** Example of a data frame (bed. example in **StratigrapheR**) providing information for each bed: id identifies each bed, l and r provide the boundaries, h the hardness, and the color is provided along with a code for lithology (S for shale, L for limestone, C for chert). The only strict convention is that l, r, and h need to be numerical values.

From such data, basic lithologs made of rectangles can be generated as a simple basis. They are the starting point for making more complicated lithologs in **StratigrapheR**. The coordinates of the points making up the rectangles can be computed through the litholog() function, which only needs the position of the boundaries of the beds, their 'hardness', and an ID. Text can be added to each bed using the bedtext() function, which can be used to include the ID or the name of the bed (e.g., id in Table 1).

The output of the litholog() function can be provided to multigons() to draw the log. A symbology for different types of rocks (or any other information that the symbology is meant to provide) can be set up using the color fill and the shading. Providing a given symbology for each polygon is performed by joining the table containing the information about each bed to a table attributing symbology to rock type. We advise the use of the left\_join() function in the dplyr package (Wickham et al., 2020) for this procedure.

•	litho ‡	col 0	density	angle *
1	S	grey30	30	180
2	L	grey90	0	0
3	С	white	10	45

```
# left_join in the dplyr package merges the symbology with the table of beds:
bed.legend <- dplyr::left_join(bed.example,legend, by = "litho")</pre>
```

^	id ÷	1 0	r ÷	h ÷	colour	litho	col ÷	density	angle
1	B1	0	1	3	grey	S	grey30	30	180
2	B2	1	3	4	grey	L	grey90	0	C
3	В3	3	4	5	black	С	white	10	45
4	B4	4	9	4	white	L	grey90	0	O
5	B5	9	11	4	white	L	grey90	0	0

## 5 Present limitations and prospects for the future

StratigrapheR, for the moment, uses the base graphics in R. This is a choice that was made in the initial development phase of the package, as the base graphics (also called traditional graphics) are easy to learn for R beginners and are relatively robust, compared to their alternative; the grid graphics (Murrell, 2012). The grid graphics are the basis for the lattice (Sarkar, 2008) and ggplot2 (Wickham, 2016) graphical packages. Grid graphics allow more sophistication than the base graphics, but at the price of a more complicated implementation (Murrell, 2012). However, grid graphics would make the entire litholog generation process more efficient, especially by using the concept of grob (which stands for GRaphical OBject). Grobs are R objects that save all the information of a plot, which can then be modified without needing to alter or rewrite the code made to generate the grobs. This would avoid any unnecessary repetition of code. Revisiting the examples in the article, you will see that the code needed for litholog generation does require writing the entire plotting functions at each plot generation or inserting them into a function. On the other hand, elements of a plot made in grid graphics can be expressed via grobs and can be reassembled to generate a modified version of the plot without explicitly making a function or repeating the code. This would further simplify drawing different parts of the same plot on several pages: if a litholog was expressed as a grob, only a few lines of codes would be needed to generate successive versions of the plot, and make them fit on different pages. For all these reasons, grobs would prove to be a key feature for future litholog generation into R. This would especially be useful to integrate lithologs in plots made by other packages, something which was not explored in this article: in the current implementation of StratigrapheR (i.e., without grobs), this would be more complicated than it could be (although it should still be possible). We hope to explore this aspect in the subsequent developments of the **StratigrapheR** package.

More generally, the difficulty of importing SVG objects into R should be discussed. With pointsvg(), only polyline and polygon objects can be imported; their color, line type, or line thickness are not taken into account. However, this is justified by the fundamental incompatibility between SVG and R graphics, whether from base graphics or grid graphics: SVG files display a wide variety of graphical parameters that are inexistent in R. Other authors have attempted to allow the complete importation of vector graphics into R (e.g., grImport (Murrell, 2009), or the vectoR package available from GitHub). These works are remarkable but require a lot more effort to use compared to pointsvg(). This comes from the fact that the only task allocated to pointsvg() is to provide coordinates of polygons and polylines. Afterward, the graphical parameters can be dealt with in R. Therefore we argue that this limitation is not by any means a flaw that will impede the use of StratigrapheR or R to deal with geological data. Furthermore, in order to work with pointsvg(), one only needs to simplify SVG objects into polygons and polylines. This procedure can be done quite easily in vector graphics software but could also be automated either in R or using SVG-related software and libraries.

Pattern fillings, often used to represent lithologies in traditional lithologs, are currently difficult to plot in R. Indeed, carbonates are often represented with a brick pattern, shales with horizontal layering, and conglomerates by a pattern of polygons to represent heterogeneous pieces. Not all of these pattern fillings are easily implementable in R at the moment, as the only user-friendly pattern is the shading (parallel lines). Rectangular pattern blocs could be generated in SVG form, imported in R using the pointsvg() function, and repeated to fill polygons.

Another useful feature that has not been implemented in **StratigrapheR** yet is a way to display 'hardness' variations within the lithological beds. The side opposite to the axis could indeed exhibit continuous variations, which would represent continuous changes in hardness, changes in topographical relief of beds in the field (which is a good indicator of hardness), but also variations of grain size or lithology. These are parameters that are critical to quantify and formalize. We therefore advocate for a community effort to come up with standards for the quantification of the hardness, topographical relief, grain size, and lithology. The way to quantify these parameters should allow to express them in discrete values along the stratigraphical depth or height. These discrete values will make up the points of the polygons symbolizing the beds, on the 'hardness'-varying side of the litholog.

The importation of the PDF documents generated by pdfDisplay() back into R, to make documents including the lithologs and providing supporting information (maps, legends, descriptions, etc.), could, in theory, be implemented using the R Markdown scheme (see Xie et al. (2018), Xie et al. (2020) and Allaire et al. (2021) that document the rmarkdown package). In practice, however, the include\_graphics() function in knitr (Xie, 2020), which is used to import PDF files in R Markdown, does not allow the selection of specific pages. This means that, for the moment, R Markdown is not well-suited for such a task. Nonetheless, this can be done using LaTeX.

**StratigrapheR**, for the moment, does not provide a library of geological features symbology, to avoid favoring specific standards of symbology that are not the norm for all geoscientists. However, we encourage the creation of different geological data formats and of their related symbology. One idea would be to have a repository for different geological symbols, grouping different versions of symbols standing for identical geological features and enabling easy download (and upload of new formats).

Finally, the definitive answer to the "from art to usable data" challenge would be to enable the importation into R of lithologs made by other software. This would be easily applicable with ad hoc software tools for which all the geological information is available in a text file. It would furthermore be conceptually possible to import computer-drawn lithologs into Geographical Information System (GIS) software such as the open-source QGIS, treat the polygons and polylines making up the litholog as spatial data, and to couple them with geological meta-data (i.e., by manually selecting these objects and providing them with identification, lithological information, etc.). This could be further facilitated by using algorithms developed for Optical Character Recognition (OCR, typically used to convert handwritten or printed text) and apply them to geological symbols. The combination of polygons, polylines, meta-data, and symbology could subsequently be used as a basis for a general-purpose litholog data format, which could then be imported in R and allow direct figure generation. With this idea, one could make software facilitating the conversion of one geological data format (e.g., hand-drawn lithologs) into this general format and then back to another format (e.g., the LAS format). The final step of this would be to improve and streamline the exchange and publication of geological data.

## 6 Summary

**StratigrapheR** explores new concepts to deal with geological data. It can serve as a strong basis for the generation of lithologs, especially facilitating the workflow when repetitive features are present. The importation of quantified data and the generation of lithologs can be refined to very simple and reproducible steps. Complex drawings can also be included. Modifying the lithologs can be automated, as the geological data can be reprocessed in R or corrected in the files used to generate the lithologs: this means that the visual output can be efficiently updated.

For the future, litholog generation in R has a strong potential to be improved: anyone willing to code in R can put a personal spin on our current work. Ultimately, all types and formats of lithologs could be imported, treated, converted, and exported efficiently, using R as a focal point for geological data processing.

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