InfiltrodiscR: an R package for infiltrometer data analysis and an experience for improving data reproducibility in a soil physics laboratory

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Abstract

This paper addresses the increasing interest and knowledge among soil physics researchers to use R, language which offers distinct advantages in terms of data reproducibility. Achieving reproducibility is a challenge in various scientific fields, including soil science, and is further driven by the demand for transparency from funding agencies and governmental institutions. Open and reproducible soil physics research can have significant positive impacts on the scientific community. Motivated by the goal of promoting open and equitable research, the authors leveraged the existing knowledge of R in a soil physics laboratory (Soil Biophysics Laboratory) and the need for a repository with common functions for infiltrometer data analysis, developed the R package infiltrodiscR. The goal of infiltrodiscR is to provide functions for the fitting of data derived from the Minidisk Infiltrometer device.

Introduction

Many soil physics researchers are unacquainted about the functionalities of the programing language R (Sousa et al. 2020). R is a is a programming language primarily used for statistical and data analysis. One main functionality that differentiates R from spreadsheet-based programs is that R scripts are text-based, making them easily shareable and reproducible, allowing to replicate analyses. The challenge of achieving reproducibility persists across various scientific disciplines, extending it to soil science as well (Correndo et al. 2023). Also, researchers in soil science, and almost every other field, are being pushed by funding agencies and governmental institutions to increase transparency and reproducibility of their work (Bond-Lamberty, Smith, and Bailey 2016). Open, accessible, reusable, and reproducible soil hydrologic research can have a significant positive impact on the scientific community and broader society (Hall et al. 2022). In this work, an R package (infiltrodiscR) is presented containing R

functions compatible with tidyverse package for infiltrometer data analysis.

Motivation

In 2023, the authors of this work joined to a program lead by Open Life Science; a community-oriented non-profit organisation that promotes open, inclusive and equitable research (Haynes 2023). In addition, the members of the Soil Biophysics laboratory (Soil Biophysics Lab 2023) already had knowledge of R but there was no repository with common functions for the infiltrometer data analysis. Based on the programming expertise of the laboratory members and the need of adoption of open and reproducible science, the R package InfiltrodiscR was developed (Acevedo and Giraldo 2023). The goal of infiltrodiscR is to provide functions for the fitting of data derived from the Minidisk Infiltrometer device. To determine the unsaturated hydraulic conductivity for a specific suction, infiltrodiscR uses the relationship between cumulative infiltration vs. time. The hydraulic conductivity of the soil $(K_{(h)})$ is calculated as the ratio of C_1 (the slope of the curve of the cumulative infiltration vs. the square root of time) and A (parameter depending on the van Genuchten parameters, the disk radius and the applied suction) based on the equation proposed by Zhang (1997).

R package description

The R package is currently hosted in GitHub. This web-based Git repository hosting service is currently used by many scientists to work in teams or collaborative projects (Bond-Lamberty, Smith, and Bailey 2016). Also, the code was deposited in Zenodo, a free service for hosting data and software that offers long-term (20-year) storage and integration with GitHub (Hall et al. 2022). The infiltrodiscR package has a DOI so it can be used as reference in publications and clearly define the software version used (Acevedo and Giraldo 2023).

To install the R package, the users need to run to following lines:

```
# install.packages("devtools")
devtools::install_github("biofisicasuelos/infiltrodiscR")
```

Data needed for running the functions are data stored in **.csv** or **.xlsx** containing columns called as follows:

- texture: soil texture according to USDA: as.character() and lowercase, for example "clay loam".
- suction: as.character() and lowercase, in this format: "2cm". Values allowed: "0.5cm","1cm","2cm","3cm","4cm","5cm","6cm", and "7cm".
- volume: volume recorded in the infiltration measurements in mL, as.numeric().
- time: time recorded in the infiltration measurements in seconds, as.numeric().

Table 1: Table 1. Selected data from the InfiltrodiscR package

texture	alpha	n/ho	2cm	4cm	6cm
sand	0.145	2.68	1.727908	0.8926213	0.4611201
loamy sand	0.124	2.28	2.428600	1.8443631	1.4006735
sandy loam	0.075	1.89	3.909913	3.9541483	3.9988836
loam	0.036	1.56	6.267384	7.5304822	9.0481388
silt	0.016	1.37	8.714378	9.8964325	11.2388254
silt loam	0.020	1.41	7.929874	9.1856010	10.6401773
sandy clay loam	0.059	1.48	4.242925	6.1530807	8.9231845
clay loam	0.019	1.31	6.644845	7.8616094	9.3011807
silty clay loam	0.010	1.23	8.511175	9.4110072	10.4059732
sandy clay	0.027	1.23	4.089288	5.3640585	7.0362184
silty clay	0.005	1.09	6.359575	6.7578953	7.1811641
clay	0.008	1.09	4.300401	4.7393888	5.2231893

Main functions:

infiltration()

This function calculates cumulative infiltration and the square root of time, using time and volume recorded based on the relationship described by Philip (1957):

$$I = C_1 t + C_2 t^{0.5}$$

vg_par()

This function returns the parameter A, *no_h* and *alpha* related to the van Genuchten parameters (Genuchten 1980), from tabulated data calculated for a radius of 2.25 cm, including 12 soil texture classes and suctions from -0.5 cm to -7 cm. Table 1 show selected data gathered from Meter Group (2023) and Carsel and Parrish (1988).

parameter_A()

This function returns the parameter A calculated from the equation based on the work developed by Zhang (1997), where the parameters A, *no_h* and *alpha* determined previously are input in the following equations described in Meter Group (2023) and Surda et al. (2019)

$$A = \frac{11.65(n^{0.1} - 1)exp[2.92(n - 1.9)\alpha h_0]}{(\alpha r_0)^{0.91}}; n \geq 1.9$$

$$A = \frac{11.65(n^{0.1} - 1)exp[7.5(n - 1.9)\alpha h_0]}{(\alpha r_0)^{0.91}}; n < 1.9$$

Practical example

First, some dummy data about infiltration and soils is created. Volume recorded in the infiltration measurements must be in mL and time in seconds. Both variables must be numeric. In order to join data (combining two datasets: infiltration and soil data), a common identifier or ID column must be present in both datasets. Soil and infiltration data must have a common column describing each unique soil and measurement. In this example, a column called soil contains measurements of "soil_a" and "soil_b" in both datasets

```r
infiltration_data <- tibble(
  soil = c(rep("soil_a",11), rep("soil_b",11)),
  time = c(0, 30, 60, 90, 120, 150, 180, 210, 240, 270, 300, # seconds
           0, 35, 65, 95, 125, 155, 185, 215, 245, 275, 305),
  volume = c(95, 89, 86, 83, 80, 77, 74, 73, 71, 69, 67, # mL
             83, 77, 64, 61, 58, 45, 42, 35, 29, 17, 15)
)

soil_data <- tibble(soil = c("soil_a", "soil_b"),
                    texture = c("sandy loam", "clay loam"), #USDA
                    suction = c("4cm","2cm"),
                    om_content = c(1,10))

head(infiltration_data,4) # check the infiltration data
```

```
# A tibble: 4 x 3
  soil    time volume
  <chr>  <dbl>  <dbl>
1 soil_a     0     95
2 soil_a    30     89
3 soil_a    60     86
4 soil_a    90     83
```

```r
soil_data # check the soil data
```

```
# A tibble: 2 x 4
  soil   texture    suction om_content
  <chr>  <chr>      <chr>         <dbl>
1 soil_a sandy loam 4cm               1
2 soil_b clay loam  2cm              10
```

Then, using the function **infiltration()** the cumulative infiltration and the square root of time are calculated. Notice that the package was coded tidy-oriented (tidyverse package is required). Also, it is recommended to use nested tibbles for data manipulation. A nested tibble stores dataframes as list-columns within another dataframe, creating a data structure with multiple layers of data. List-columns are particularly useful for researchers because the elements (e.g., fitting models and estimated values) of the list-columns can be easily processed by iteratively applying a function for estimation and summary to each element of the list-column using the functional programming functions (e.g., map()) in the purrr package (Lee, Sriutaisuk, and Kim 2019)

```
infilt_cum_sqrt <-
infiltration_data %>%
group_by(soil) %>% # grouped calculation by soil
nest() %>%
mutate(data = map(data, ~ infiltrodiscR::infiltration(.), data = .x))

infilt_cum_sqrt # nested tibble
```

```
# A tibble: 2 x 2
# Groups:   soil [2]
  soil    data
  <chr>   <list>
1 soil_a <tibble [11 x 5]>
2 soil_b <tibble [11 x 5]>
```

The nested tibble has the infiltration calculation for each soil. For details of **infilt_cum_sqrt**, the **unnest()** function can be used

```
infilt_cum_sqrt %>%
  unnest(data) %>%
  head(6) # check
```

```
# A tibble: 6 x 6
# Groups:   soil [1]
  soil    time volume sqrt_time volume_infiltrated infiltration
  <chr>  <dbl>  <dbl>     <dbl>              <dbl>        <dbl>
1 soil_a     0     95      0                     0            0
2 soil_a    30     89      5.48                  6         0.38
3 soil_a    60     86      7.75                  9         0.57
4 soil_a    90     83      9.49                 12         0.75
5 soil_a   120     80     11.0                  15         0.94
6 soil_a   150     77     12.2                  18         1.13
```

Now the soil data can be joined to the infiltration data and the Van Genuchten parameters can be obtained. It is mandatory to have a column called **texture** and another **suction**

```
infilt_cum_sqrt %>%
  left_join(soil_data) %>%
  infiltrodiscR::vg_par()
```

```
Joining with `by = join_by(soil)`
Joining with `by = join_by(texture)`
```

```
# A tibble: 2 x 8
# Groups:   soil [2]
  soil   data               texture    suction om_content alpha  n_ho value_A
  <chr>  <list>             <chr>      <chr>         <dbl> <dbl> <dbl>   <dbl>
1 soil_a <tibble [11 x 5]>  sandy loam 4cm               1 0.075  1.89    3.95
2 soil_b <tibble [11 x 5]>  clay loam  2cm              10 0.019  1.31    6.64
```

The hydraulic conductivity of the soil K at a specific suction is calculated as:

$$K_{(h)} = \frac{C_1}{A}$$

Parameter C_1 is calculated fitting a polynomial function of the second degree ($y = ax2+b$), where a is parameter C_1, x is the square root of time and y is the cumulative infiltration calculated previously. For this step, we use the package broom and base R. The column estimate corresponds to the parameter C_1.

```
processed_data <-
infilt_cum_sqrt %>%
  left_join(soil_data) %>%
  infiltrodiscR::vg_par() %>%
    mutate(
    fit = map(data,
              ~ lm(infiltration ~ poly(sqrt_time, 2, raw = TRUE),
                   data = .x)), #polynomial function
    tidied = map(fit, broom::tidy) #coefficients
  ) %>%
  unnest(tidied) %>%
filter(term == "poly(sqrt_time, 2, raw = TRUE)2") %>% #slope
rename(C1 = estimate)
```

```
Joining with `by = join_by(soil)`
Joining with `by = join_by(texture)`
```

Finally, the hydraulic conductivity of the soil K is calculating using the parameter C_1 and A. If seconds and mL were used as inputs for infiltration data, the units of K are cm/s.

```
processed_data %>%
  infiltrodiscR::parameter_A() %>%
  mutate(K_h = C1 / parameter_A) %>%
  select(soil, texture, suction, K_h)
```

```
# A tibble: 2 x 4
# Groups:   soil [2]
  soil   texture    suction       K_h
  <chr>  <chr>      <chr>        <dbl>
1 soil_a sandy loam 4cm       0.000638
2 soil_b clay loam  2cm       0.00212
```

Using this tidy-oriented approach, it is simple to complement the functions presented with plotting.

```
infiltration_plot <-
infilt_cum_sqrt %>%
  left_join(soil_data) %>%
  mutate(plot = map2(
    data, soil,
    ~ ggplot(data = .x, aes(x = sqrt_time, y = infiltration)) +
      ggtitle(glue::glue("Soil : {soil}
                  Suction : {suction}")) +
      stat_smooth(method='lm', formula = y~poly(x,2)) +
      geom_point() +
      theme_bw())))
```

```
Joining with `by = join_by(soil)`
```

```
patchwork::wrap_plots(infiltration_plot$plot, ncol = 2)
```
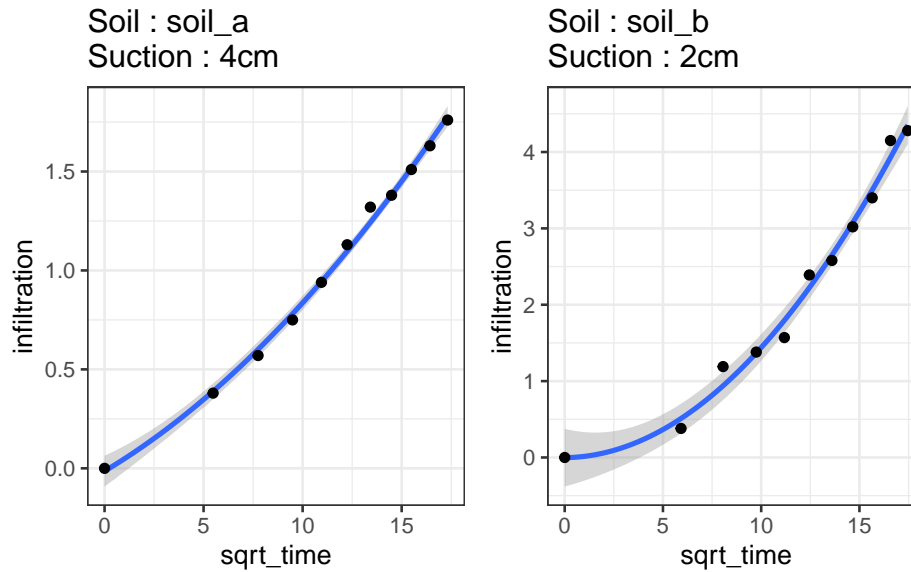
Conclusions and future work

The learning curve in R programming and open science practices is not the same for every researcher, nor is it a dedicated line of research in graduate programs dedicated to soil physics. Therefore, this experience in creating an R package homogenizing the data analysis methodology in a laboratory shows that if there is interest in developing this approach, further advances in collaboration and reproducibility can be made. Also, based on the R background of the users of the package, the functions were developed using the same the grammar, pipelines, and data visualization practices of tidyverse, which allowed it to be easily adopted by the researchers.

Acknowledgements

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