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Optimization of SIMS-based stable isotope measurements with regression diagnostics

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Processing math: 100%

SIMS in Geosciences

Increasing the spatial resolution of isotope analysis in Earth science studies has/will expand our understanding of the processes that shape our planet.

Highly resolved isotope analysis with Secondary Ion Mass Spectrometry (SIMS) has been applied to address questions concerning:

- sediment diagenesis
- biomineralization
- proxy development
- cosmochemistry

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R package point::functions

R package under development on github: https://github.com/MartinSchobben/point

```
# Install point from GitHub:
# install.packages("devtools")
devtools::install_github("https://github.com/MartinSchobben/point", build_vignettes = TRUE)
```

Main functions of the package

- reading pulsed ion count data
- process ion count data to accommodate machine-specific systematic biases
- calculate predictive (Poisson) and descriptive statistics of single ions and isotope ratios (random bias)
- perform diagnostics on stability of individual analysis

The package works but is still “work-in-progress”

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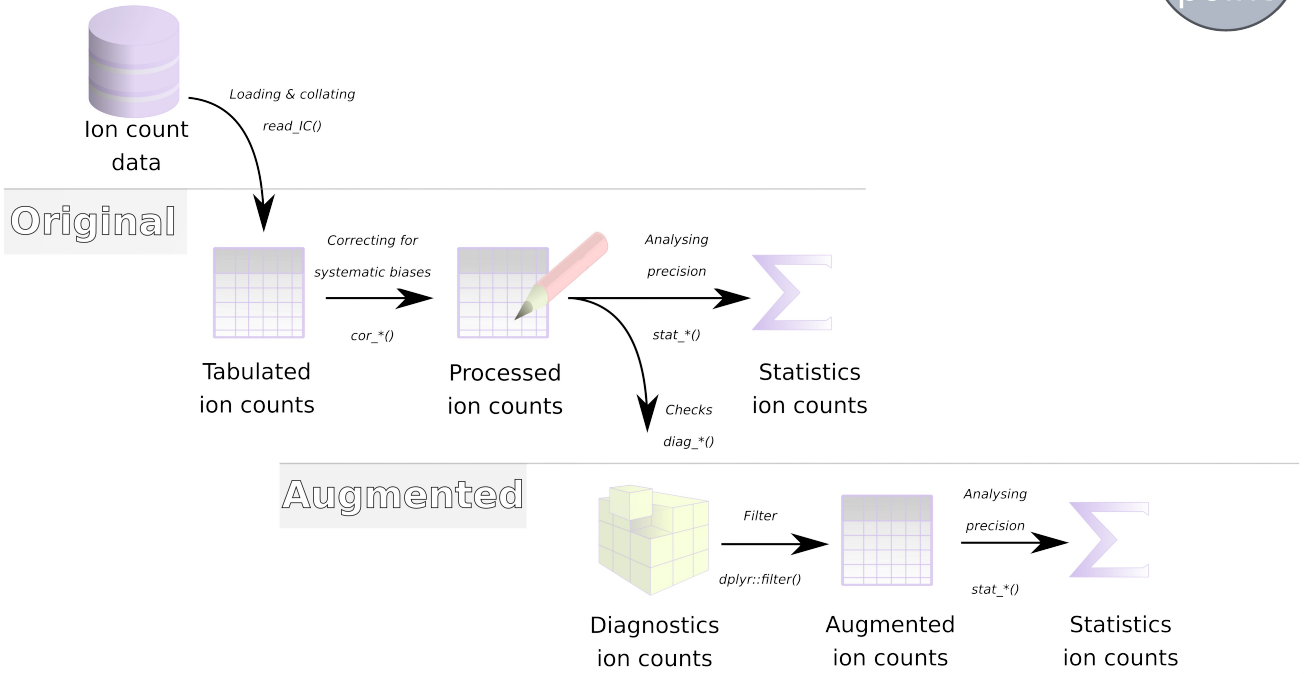
R package point::functions



Example: calculating internal precision

```
# load package
library(point)
# Raw data containing 13C and 12C counts on carbonate
tb.rw <- read_IC(point_example("2018-01-19-GLENDON"))

# Processing raw ion count data
tb.pr <- cor_IC(tb.rw,
                N = N.rw,
                t = t.rw,
                Det = det_type.mt,
                deadtime = 44,
                thr_PHD = 50)

# Descriptive an predictive statistics for 13C/12C ratios
tb.R <- stat_R(tb.pr,
               Xt = Xt.pr,
               N = N.pr,
               species = species.nm,
               ion1 = "13C",
               ion2 = "12C",
               sample.nm,
               file.nm,
               latex = TRUE)
```

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Example: calculating internal precision

sample.nm	R	n	$\bar{R}$	s_R	ϵ_R (‰)	$s_{\bar{R}}$	$\epsilon_{\bar{R}}$ (‰)	$\hat{s}_R$	$\hat{\epsilon}_R$ (‰)	$\hat{s}_{\bar{R}}$	$\hat{\epsilon}_{\bar{R}}$ (‰)	χ^2
Belemnite, Indium	$^{13}C/^{12}C$	3900	0.01097	0.001020	93.0	1.63e-05	1.49	0.001017	92.8	1.63e-05	1.49	1.004
Belemnite, Indium	$^{13}C/^{12}C$	3900	0.01097	0.000777	70.8	1.24e-05	1.13	0.000769	70.1	1.23e-05	1.12	1.020
Belemnite, Indium	$^{13}C/^{12}C$	3900	0.01099	0.000731	66.5	1.17e-05	1.07	0.000721	65.5	1.15e-05	1.05	1.030
W12, Indium (W12_Indium_1_1)	$^{13}C/^{12}C$	4000	0.01077	0.000759	70.5	1.20e-05	1.11	0.000759	70.5	1.20e-05	1.11	1.000
W12, Indium (W12_Indium_1_10)	$^{13}C/^{12}C$	4000	0.00503	0.318830	63447.2	5.04e-03	1003.19	0.318614	63404.3	5.04e-03	1002.51	1.001
W12, Indium (W12_Indium_1_10)	$^{13}C/^{12}C$	4000	0.01094	0.000916	83.8	1.45e-05	1.32	0.000919	84.0	1.45e-05	1.33	0.996

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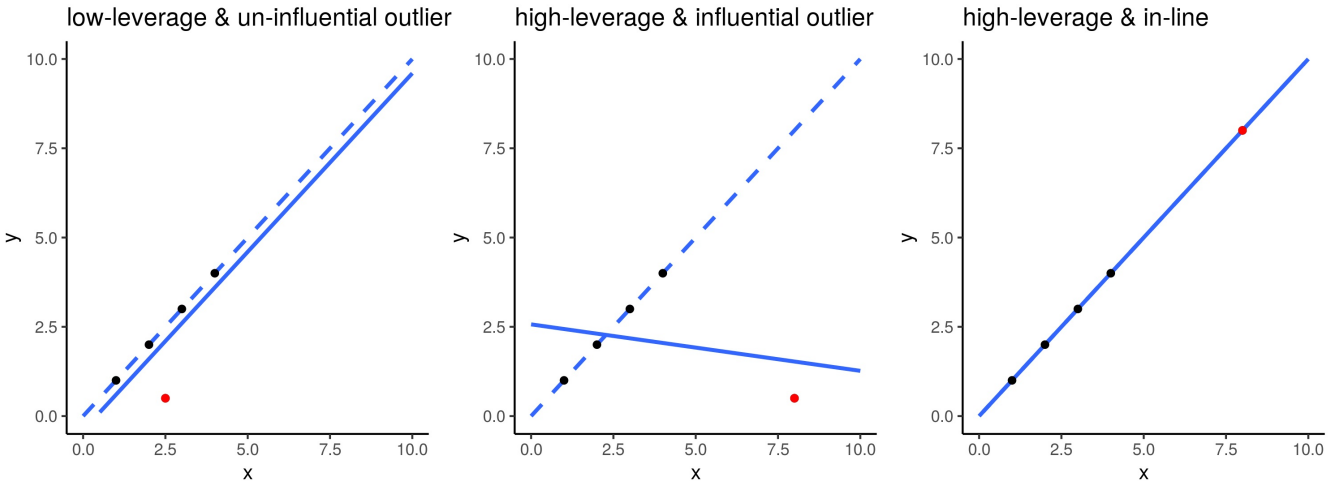
Regression diagnostics



Cook's Distance measure estimates influence based on leverage and outlyingness

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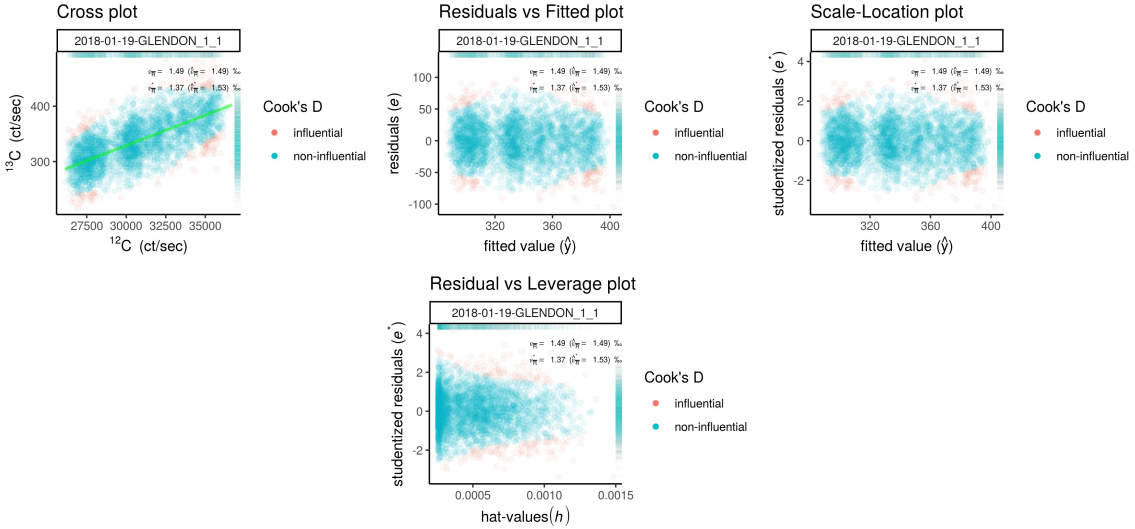
Regression diagnostics



Regression diagnostics of a single analysis on carbonate $^{13}C/^{12}C$ with a NanoSIMS 50L

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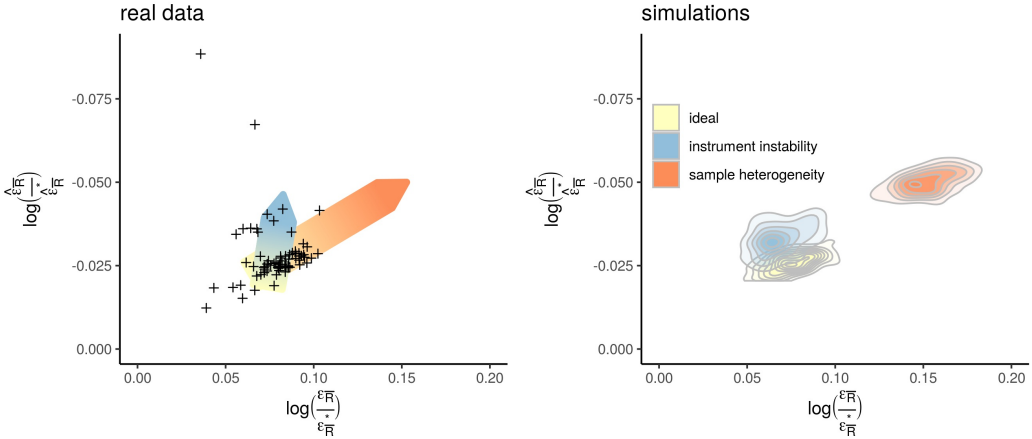
Detecting source(s) of unaccounted biases

Comparing descriptive and predictive statistics of the original and augmented datasets yields information about the source of bias.



Example of 73 analyses on carbonate $^{13}C/^{12}C$ with a NanoSIMS 50L (real data) and simulated data

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Summary

1) R package for reading, processing and analysing ion count data

2) Regression diagnostics might identify sample heterogeneity/instrument instability

For more information visit: https://github.com/MartinSchobben/point

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Acknowledgements

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Allaire, JJ, Yihui Xie, Jonathan McPherson, Javier Luraschi, Kevin Ushey, Aron Atkins, Hadley Wickham, Joe Cheng, Winston Chang, and Richard Iannone. 2019. *Rmarkdown: Dynamic Documents for R*. https://github.com/rstudio/rmarkdown.

Xie, Yihui. 2015. *Dynamic Documents with R and Knitr*. 2nd ed. Boca Raton, Florida: Chapman; Hall/CRC. https://yihui.org/knitr/.

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Xie, Yihui, J.J. Allaire, and Garrett Grolemund. 2018. *R Markdown: The Definitive Guide*. Boca Raton, Florida: Chapman; Hall/CRC. https://bookdown.org/yihui/rmarkdown.