

robstack, a fast R package to read, process and plot NOAA/GML ObsPack

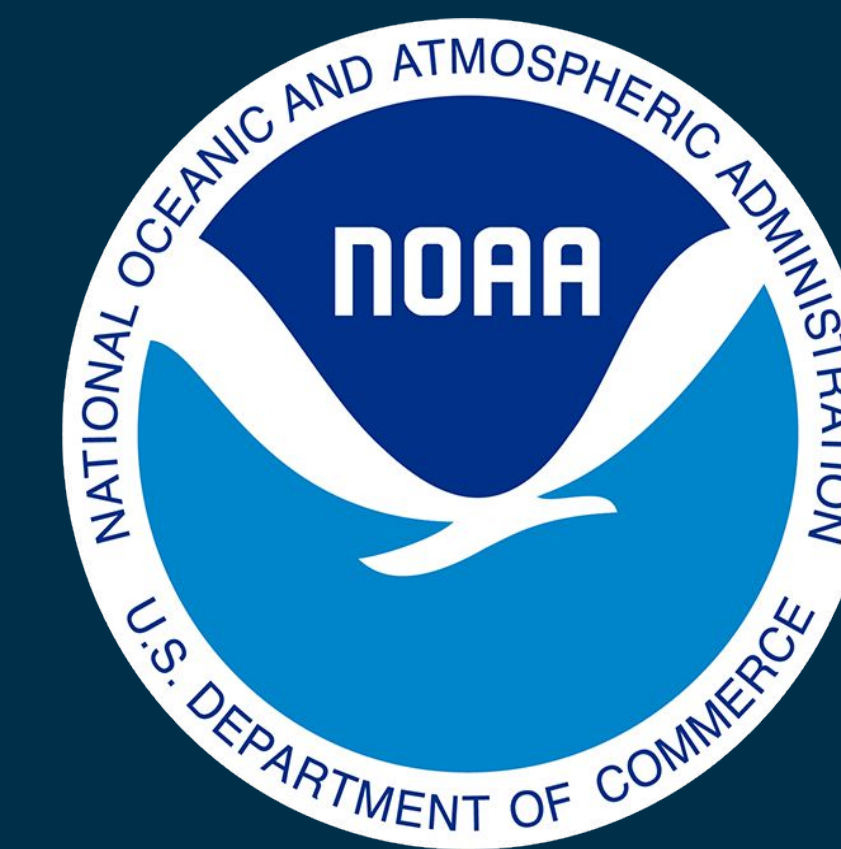
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Motivation and goals

- Methane is a greenhouse gas (GHG) that affects the Earth's radiative forcing and consequently, the climate system.
- The NOAA Global Monitoring Laboratory (GML) manages a global network of atmospheric observations compiled and delivered to the public as ObsPack CH₄ GLOBALVIEW+.
- We developed the R package **robstack**, which reads and processes NOAA/GML ObsPack

Ok, but why?

We are studying the impact of COVID19 on CH₄ posterior emissions. We use atmospheric inversions to estimate posterior methane emissions (e.g. Hu et al., 2017; 2019).

$$s = s_p + (HQ)^T * (HQH^T + R)^{-1} * (z - Hs_p)$$

- z vector of measurements
- H matrix that describes the relationship between measurements and the unknown fields (*footprints*)
- R is the covariance matrix of the model-data mismatch errors
- s_p is the prior estimate of s
- Q is a prior error covariance matrix of emissions

robstack provides z and inputs for H (not only *flask*, also *insitu*!)

System Requirements

- **robstack** imports data.table (Dowle & Srinivasan, 2021), which is basically C + OpenMP (super fast! check <https://h2oai.github.io/db-benchmark/>)
- Also imports lubridate (Grolemund, 2011), cptcity (Ibarra-Espinosa 2018), and other base packages (R Core Team 2022).
- **robstack** can be installed in any OS (there is no need of conda 🐍)

Application for tower-insitu

Installation and summary of the data

```
remotes::install_github("ibarraespinoza/robstack")
obs <- "obspack_ch4_1_GLOBALVIEWplus/data/txt"
index <- obs_summary(obs = obs)
```

```
Number of files of index: 362
      sector      N
1: aircraft-pfp  40
2: aircraft-insitu 11
3: flask       101
4: surface-insitu 124
5: aircore      1
6: surface-pfp  33
7: tower-insitu  51
8: shipboard-insitu 1
9: Total sectors 362
Detected 136 files with agl
Detected 226 files without agl
```

- 1) The object index is a table with path for each ObsPack file, including altitude AGL and sector.
- 2) Read and add metadata information as columns. The object `df` contains all observations, including laboratory and respective scales. Then we can filter by space and time.

```
df <- obs_read(index = index, categories = "tower-insitu")
df[altitude_final < 10 & longitude > -170 & longitude < -50 &
  latitude > 10 & latitude < 80 & year ==% 2020]
```

- 3) Time. convert from seconds to time POSIXct, identifying intervals and ending and starting times.

```
df2 <- obs_addtime(df)
```

- 4) Plot, where we can control groups to plot. For site "LEF", higher observations are found closer to surface on Fig 1, $n = 104870$

```
obs_plot(dt = df2[site_code=="LEF"], time = "timeUTC", yfactor = 1e9,
  cex = 0.5, ylab = expression(CH[4]~ppb), colu = "altitude_final",
  pal = "mpl_viridis", n = c(122, 30, 396))
```

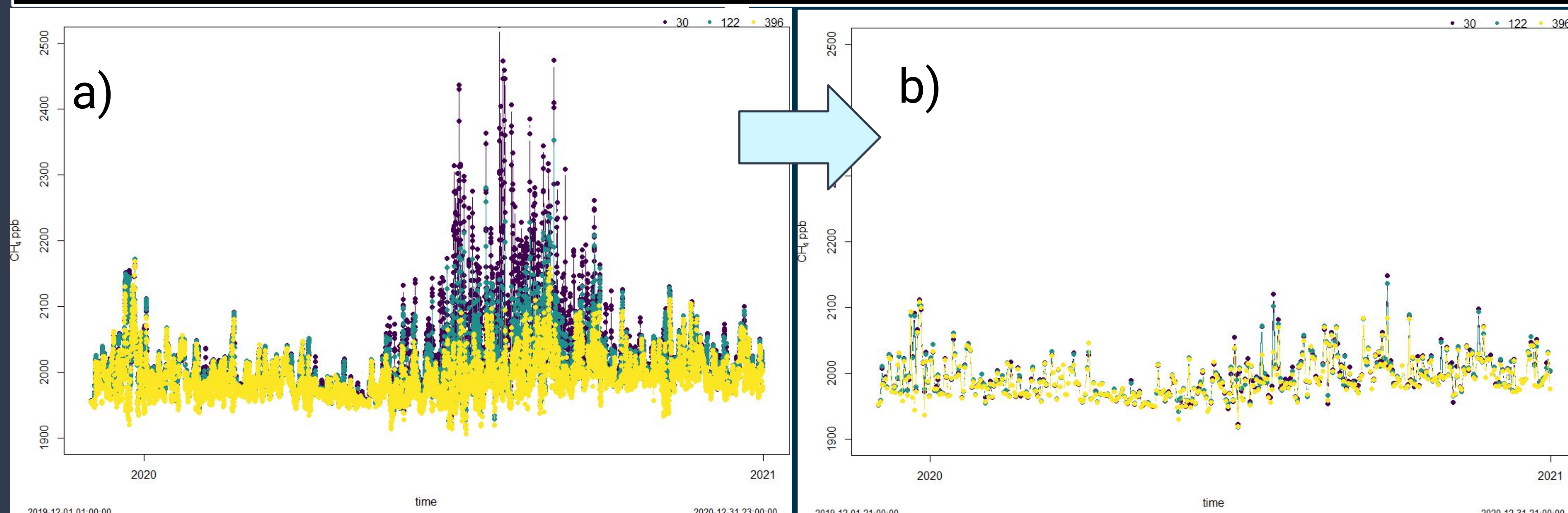


Figure 1. a) Observations of CH₄ for the site LEF by altitude and b) the same but filtered.

- 5) First we cut UTC time every 2 hours. We are interested in daily data 2-3pm local time (LT). LT is obtained via metadata, or calculated using the following formula. Then we select local hours 2-3pm.

$$LT = UTC + longitude/15 * 60 * 60$$

```
df2 <- obs_addtime(df)
df2$timeUTC <- cut(x = df2$timeUTC + 3600,
  breaks = "2 hour")
df3 <- obs_addtime(df2) ; df3 <- df3[1h %in% 14:15]
df4 <- obs_agg(dt = df3, gby = "mean", cols =
  c("value", "latitude", "longitude", "type_altitude",
  "dif_time", "site_utc2lst"), byalt = TRUE)
df5[, max_altitude := max(altitude_final, na.rm = TRUE),
  by = site_code]
```

- 6) Now, as there are many observations with the same time with different values. Then, we need to aggregate the data by time, lab, scale, site code and altitude. Then, the new plot on 1b) with 4394 observation has same pattern as Fig 1a), with 104870.

- 7) We need to identify the max altitude by site and select the highest

- 8) The data can be save as a master file, with all information, and the receptor, which the list of receptors. Saving the master is done including a **YAML** header.

```
obs_write(dt = df5, notes = "tower 2020",
  out = "tower_2020.csvy")
```

- 9) Saving the receptor data is similar, but the format is .txt and it is done by sector and type of altitude, AGL or ASL.

```
re<-df5[altitude_final == max_altitude,
  c("site_code", "year", "month", "day",
  "hour", "minute", "second", "latitude",
  "longitude", "altitude_final",
  "type_altitude", "year_end", "month_end",
  "day_end", "hour_end", "minute_end",
  "second_end")]
re[, af:= round(receptor$altitude_final)]
re <- obs_format(re)
```

- 10) At this point HYSPLIT is run following Hu et al (2023) to generate footprints. The last step check the the NetCDF footprints and write the inputs to run the inverse model. More details in Ibarra-Espinosa and Hu (2023)

```
tf <- obs_invfiles(master = df5,
  path = "path", Type = "continuous",
  SubType = "ground",
  Surface_Elev = master$max_altitude)
```

References

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