NMF Final (Only nndsvd 5 component without ozone)

William Zhang, Eva, Jerry, Meredith

2025-01-24

```r
# load the packages
library(NMF)
library(tidyverse)
library(grid)
library(gridExtra)
library(readxl)
library(circular)
library(lwgeom)
library(units)
```

Procedure

1. Remove hourly observation with missing observation for any chemical
2. Remove background noise level using min values (except for chemicals with minimum value < 2*LOD and maximum value > 100*LOD)
3. Zero values are converted to a random value between 0 and 0.5*LOD
4. Normalize using min and max
5. Remove Ozone (wouldn't affect # of obs.)

Reading the data

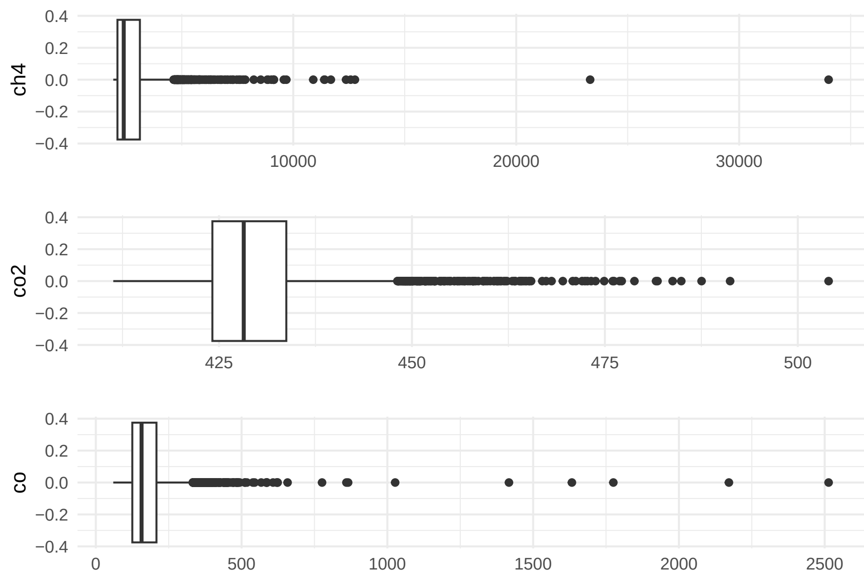
```r
hourly_data <- readRDS("../DataProcessing/Trailer_hourly_merge_20240905.rds")
```

```r
# PROCEDURE STEP 1:
hourly_data <- hourly_data %>% rename('co2' = 'co2_ppm')

vocs <- c("ethane", "ethene", "propane", "propene",
                                        "1_3-butadiene", "i-butane", "n-butane",
                                        "acetylene", "cyclopentane", "i-pentane",
                                        "n-pentane", "n-hexane", "isoprene", "n-heptane",
                                        "benzene", "n-octane", "toluene", "ethyl-benzene",
                                        "m&p-xylene", "o-xylene")


non_vocs <- c('ch4', 'co2', 'co', 'h2s', 'so2', 'nox', 'o3')

# remove row with missing obs for any chemical
hourly_nona <- hourly_data %>%
  select(any_of(c('day', 'time_utc', vocs, non_vocs, 'wdr_deg', 'wsp_ms'))) %>%
  na.omit()
```

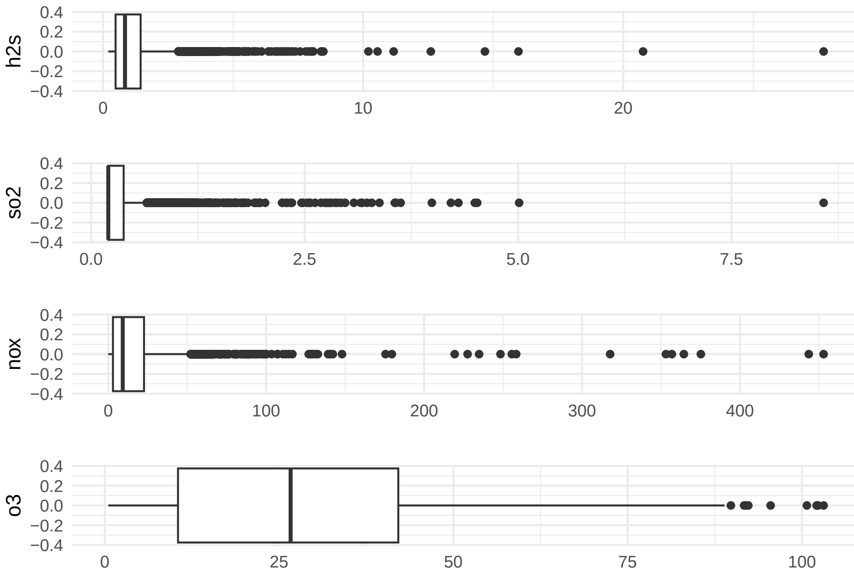
```
# retrieving the vocs, removing everything else except the vocs
hourly_vocs <- hourly_nona %>% select(any_of(vocs))

# retrieving the non-vocs: co2_ppm, nox, ch4, h2s, so2, o3
# double check this
hourly_non_vocs <- hourly_nona %>% select(any_of(non_vocs))

hourly_full_nona <- cbind(hourly_non_vocs, hourly_vocs)

# retrive a vector of yearmonth
hourly_dates <- hourly_nona %>%
  mutate(yearmonth = substring(day, 0, 7)) %>%
  pull(yearmonth)
```

Data visualisation

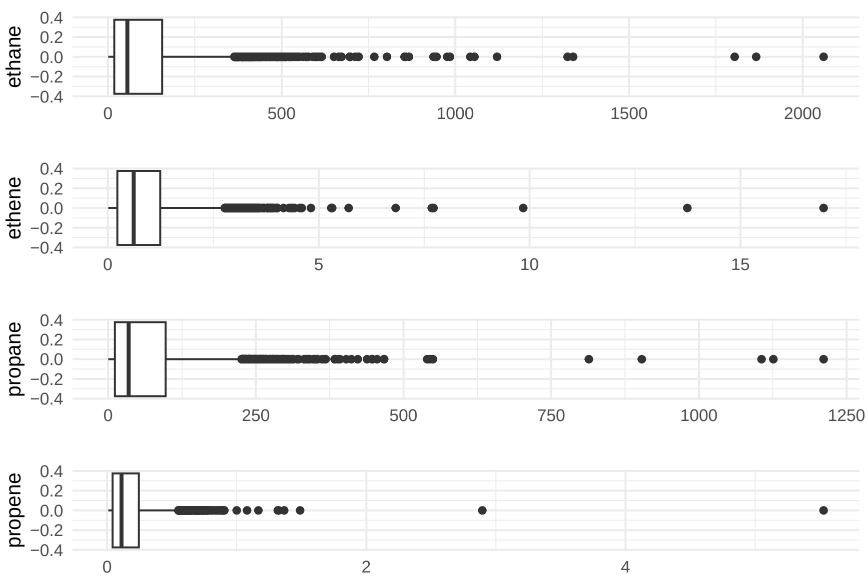
- Boxplots of the hourly concentrations non-voc

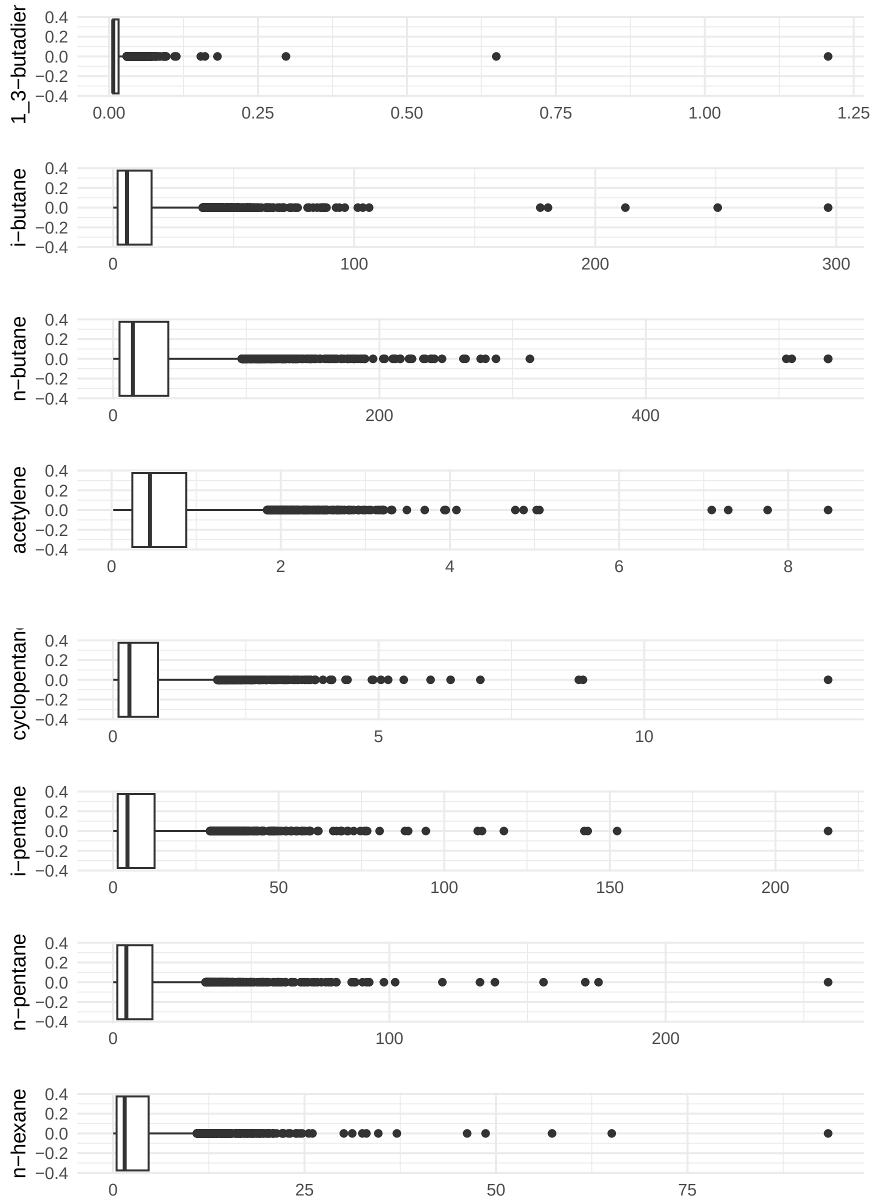


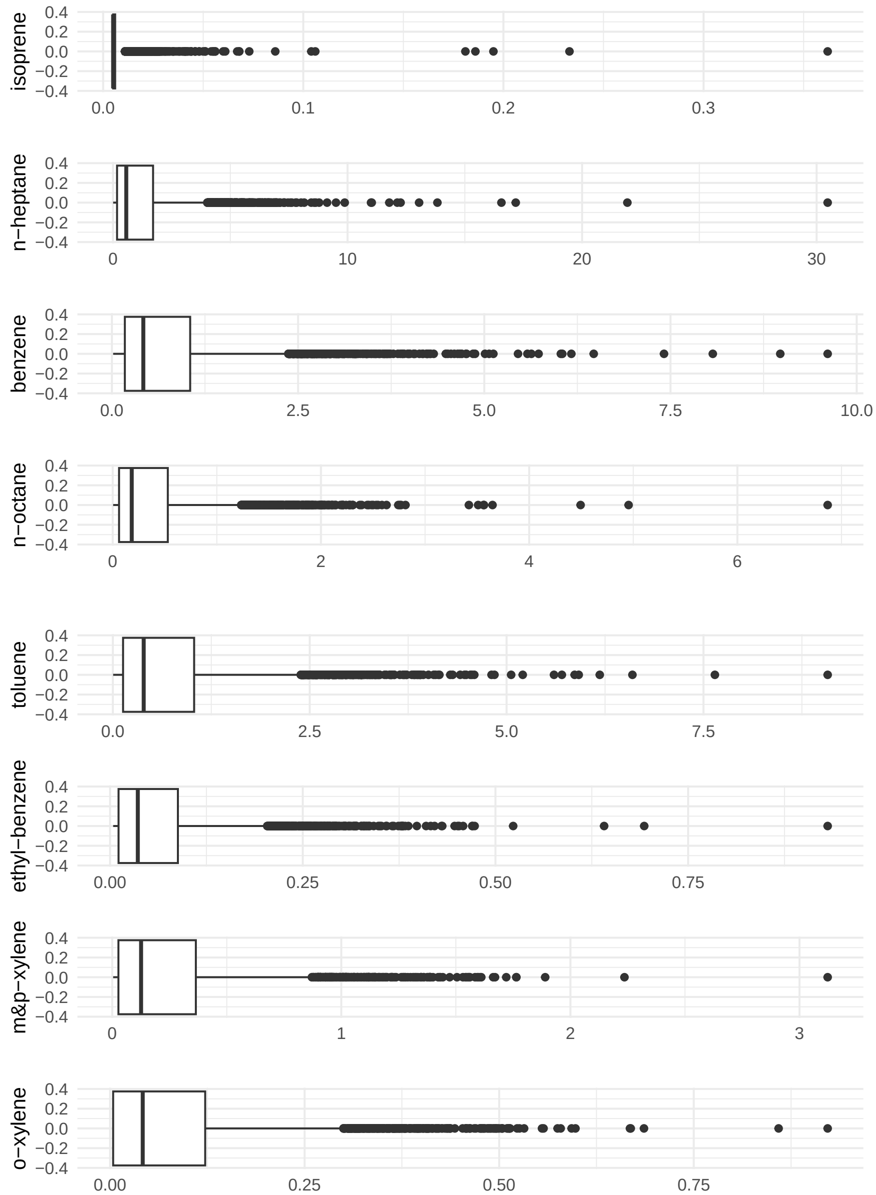
- Boxplots sulfur compounds, NOx, ozone



- Boxplots VOCs




1_3−butadier
i−butane
n−butane
acetylene
cyclopentan
i−pentane
n−pentane
n−hexane
0.00
0.25
0.50
0.75
1.00
1.25
0
100
200
300
400
2
4
6
8
5
10
50
150
25
75
0.4
0.2
0.0
−0.2
−0.4



Data pre-processing

Step 1: limits of detection

- STEP 1: Limits of detection

```
# Define LOD for each chemical
LOD_non_voc <- c('ch4' = 0.9,
                 'co2' = 0.0433,
                 'co' = 40,
                 'h2s' = 0.4,
                 'so2' = 0.4,
                 'nox' = 0.05,
                 'o3' = 1)

# LOD_voc_monthly <- read_csv('../data/LNM_VOC_LOD_Rounded.csv') %>% select(-1)
```

```r
#
# # extract the yearmonth from date variables
# LOD_voc_monthly <- LOD_voc_monthly %>%
#   mutate(yearmonth = strftime(as.POSIXct(start_date, format = '%Y-%m-%d %H:%M:%S',
#                                          tz = 'UTC'), '%Y-%m'))
#
# LOD_voc_monthly <- LOD_voc_monthly %>%
#   select(-c(start_date, end_date)) %>%
#   select(!any_of(ends_with('half_ldl')))
#
# colnames(LOD_voc_monthly) <- str_replace_all(names(LOD_voc_monthly), '_ldl', '')

LOD_voc_avg <- read_xlsx('../data/LNM_VOC_Uncertainties.xlsx', skip = 1)
LOD_voc_avg <- LOD_voc_avg %>%
  select(1, 4) %>%
  rename('LOD' = 2, 'chemical' = 1) %>%
  head(20)
```

Step 2: Background correction

- STEP 2: Background correction

```
##           ch4          co2           co          h2s          so2
##      1928.000      411.300       59.910        0.200        0.200
##           nox           o3       ethane       ethene      propane
##         0.025        0.500        0.916        0.011        0.224
##       propene 1_3-butadiene     i-butane     n-butane    acetylene
##         0.009        0.007        0.035        0.090        0.019
##  cyclopentane     i-pentane    n-pentane     n-hexane     isoprene
##         0.005        0.038        0.042        0.021        0.005
##     n-heptane      benzene     n-octane      toluene ethyl-benzene
##         0.004        0.017        0.004        0.004        0.004
##    m&p-xylene     o-xylene
##         0.004        0.004
```

- Summary statistics of backgrounds and extremes

```r
get_info <- function(column) {
  N <- length(column)
  background <- quantile(column, 0)
  quantile1 <- quantile(column, 0.01)
  quantile99 <- quantile(column, 0.99)
  n_background <- sum(column == background)
  max <- max(column)
  return(c(N, quantile1, quantile99, max, background, n_background))
}

info_table <- hourly_full_nona %>%
  reframe(across(everything(), ~ get_info(.x)))

info_table <- info_table %>%
  mutate(rownames = c('N', '1st percentile', '99th percentile', 'Max',
                      'Background', '# Background')) %>%
  pivot_longer(-rownames) %>%
  pivot_wider(names_from = rownames, values_from = value)
```

```r
knitr::kable(info_table)
```

name	N	1st percentile	99th percentile	Max	Background	# Background
ch4	4788	1962.98700	6286.12400	34010.900	1928.000	1
co2	4788	416.47870	460.62260	503.990	411.300	1
co	4788	84.23050	442.08860	2513.440	59.910	1
h2s	4788	0.20000	5.20986	27.700	0.200	829
so2	4788	0.20000	1.78686	8.578	0.200	3266
nox	4788	0.22974	89.72371	452.959	0.025	2
o3	4788	0.50000	76.02600	103.100	0.500	259
ethane	4788	1.84422	526.44700	2060.000	0.916	1
ethene	4788	0.01100	3.50826	16.970	0.011	163
propane	4788	0.84674	300.79000	1211.000	0.224	1
propene	4788	0.00900	0.69739	5.528	0.009	411
1_3-butadiene	4788	0.00700	0.05900	1.207	0.007	3357
i-butane	4788	0.15148	60.89400	296.600	0.035	1
n-butane	4788	0.37248	166.52100	536.900	0.090	1
acetylene	4788	0.04900	2.61304	8.471	0.019	2
cyclopentane	4788	0.00500	3.06899	13.460	0.005	96
i-pentane	4788	0.10987	49.60210	215.900	0.038	1
n-pentane	4788	0.10487	55.95980	258.800	0.042	1
n-hexane	4788	0.04300	18.17780	93.360	0.021	2
isoprene	4788	0.00500	0.03313	0.362	0.005	2816
n-heptane	4788	0.01500	6.57669	30.470	0.004	5
benzene	4788	0.02800	3.78693	9.610	0.017	3
n-octane	4788	0.00400	2.00839	6.867	0.004	100
toluene	4788	0.01300	3.52165	9.077	0.004	11
ethyl-benzene	4788	0.00400	0.31613	0.931	0.004	918
m&p-xylene	4788	0.00400	1.29156	3.123	0.004	851
o-xylene	4788	0.00400	0.45700	0.922	0.004	1330

- STEP 2 processing continued: background correction
- adjustments that were made according to paper: Gunnar's paper section 2.2 and Guha 3.3
- Check whether chemical has background noise level that needs to be removed
- NO ADJUSTMENT if minimum value < 2xLOD and maximum value > 100xLOD

```r
adjusting_neg_bg_from_lod <- function(chemical, LOD, background, hourly_data){
    # get min and max
    min_value <- min(hourly_data[chemical], na.rm = TRUE)
    max_value <- max(hourly_data[chemical], na.rm = TRUE)
    # if min less than double LOD or max > 100 times LOD
    # adjust to -100 (for entire column???)
    if (min_value < 2 * LOD & max_value > 100 * LOD ){
      return (0)
    }
  return (background)
}
```

- Check if background is negligible for non voc
- merge background and LOD

```r
background_lod_non_voc <- tibble(chemical = non_vocs,
                                 LOD = LOD_non_voc,
                                 background = unname(background_levels[non_vocs]))
adjusted_background_non_voc <- background_lod_non_voc %>%
  rowwise() %>%
  mutate(min = min(hourly_full_nona[chemical], na.rm = TRUE),
         LODx2 = 2 * LOD,
         criterion1 = min(hourly_full_nona[chemical], na.rm = TRUE) < 2 * LOD,
         max = max(hourly_full_nona[chemical], na.rm = TRUE),
         LODx100 = 100 * LOD,
         criterion2 = max(hourly_full_nona[chemical], na.rm = TRUE) > 100 * LOD,
         adjusted_background = adjusting_neg_bg_from_lod(chemical, LOD, background,
                                                         hourly_full_nona))
```

- Check if background is negligible for voc
- merge background and LOD

```r
background_lod_voc <- LOD_voc_avg %>%
  left_join(tibble(chemical = setdiff(names(background_levels), non_vocs),
                   background = background_levels[setdiff(names(background_levels),
                                                           non_vocs)]))
adjusted_background_voc <- background_lod_voc %>%
  rowwise() %>%
  mutate(min = min(hourly_full_nona[chemical], na.rm = TRUE),
         LODx2 = 2 * LOD,
         criterion1 = min(hourly_full_nona[chemical], na.rm = TRUE) < 2 * LOD,
         max = max(hourly_full_nona[chemical], na.rm = TRUE),
         LODx100 = 100 * LOD,
         criterion2 = max(hourly_full_nona[chemical], na.rm = TRUE) > 100 * LOD,
         adjusted_background = adjusting_neg_bg_from_lod(chemical, LOD, background,
                                                         hourly_full_nona))
```

- create dataset with background removed

```r
# So now we have the adjusted background concentrations
hourly_nona_bgrm <- hourly_full_nona %>%
  mutate(across(adjusted_background_non_voc$chemical,
                ~  .x - adjusted_background_non_voc$adjusted_background[
                    adjusted_background_non_voc$chemical == cur_column()]))
hourly_nona_bgrm <- hourly_nona_bgrm %>%
  mutate(across(adjusted_background_voc$chemical,
                ~  .x - adjusted_background_voc$adjusted_background[
                    adjusted_background_voc$chemical == cur_column()]))
```

- check number of 0 values per compound

```r
# look at zero values
colSums(hourly_nona_bgrm == 0)
```

```
##          ch4          co2           co          h2s          so2
##            1            1            1          829         3266
##          nox           o3       ethane       ethene      propane
##            0            0            1            0            1
##      propene 1_3-butadiene     i-butane     n-butane    acetylene
##            0         3357            1            1            0
##   cyclopentane    i-pentane    n-pentane     n-hexane     isoprene
```

```
##              0             1             1             2          2816
##      n-heptane       benzene      n-octane       toluene ethyl-benzene
##              0             0             0             0             0
##     m&p-xylene       o-xylene
##              0             0
```

Step 3: Replace zero with random value between 0 and 0.5*LOD

- STEP 3: replace zero values with random values between 0 and 0.5xLOD

```
set.seed(123)
replace_zero_with_random <- function(column, name, LOD_df){
  LOD <- LOD_df$LOD[LOD_df$chemical == name]
  column <- if_else(column == 0, round(runif(length(column), 0, 0.5 * LOD), 3), column)
  return (column)
}

hourly_nona_bgrm_zerorepl <- hourly_nona_bgrm %>%
  mutate(across(adjusted_background_non_voc$chemical,
                ~ replace_zero_with_random(.x, cur_column(), adjusted_background_non_voc)))

hourly_nona_bgrm_zerorepl <- hourly_nona_bgrm_zerorepl %>%
  mutate(across(adjusted_background_voc$chemical,
                ~ replace_zero_with_random(.x, cur_column(), adjusted_background_voc)))
```

Step 4: Normalize

- STEP 4: Normalize the measurements

```
#normalizing function
normalize_column <- function(column){
  background <- quantile(column, 0)
  max <- quantile(column, 1) # this could be adjusted
  return ((column - background)/(max - background))
}
```

```
# normalize all
hourly_nona_bgrm_zerorepl_norm <- as_tibble(sapply(as.list(hourly_nona_bgrm_zerorepl),
                                                   normalize_column))
#normalize the NON_VOC
summary(hourly_nona_bgrm_zerorepl_norm)
```

```
##       ch4                co2                co                 h2s
##  Min.   :0.00000   Min.   :0.0000   Min.   :0.00000   Min.   :0.00000
##  1st Qu.:0.00579   1st Qu.:0.1384   1st Qu.:0.02592   1st Qu.:0.01022
##  Median :0.01460   Median :0.1823   Median :0.03884   Median :0.02335
##  Mean   :0.02683   Mean   :0.2000   Mean   :0.04761   Mean   :0.03501
##  3rd Qu.:0.03720   3rd Qu.:0.2418   3rd Qu.:0.05970   3rd Qu.:0.04525
##  Max.   :1.00000   Max.   :1.0000   Max.   :1.00000   Max.   :1.00000
##       so2                 nox                  o3              ethane
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.00000   Min.   :0.000000
##  1st Qu.:0.007878   1st Qu.:0.006534   1st Qu.:0.09747   1st Qu.:0.008385
##  Median :0.015994   Median :0.020262   Median :0.25487   Median :0.026671
##  Mean   :0.026287   Mean   :0.036440   Mean   :0.26676   Mean   :0.050992
##  3rd Qu.:0.023633   3rd Qu.:0.049978   3rd Qu.:0.40546   3rd Qu.:0.075375
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.00000   Max.   :1.000000
```

```
##      ethene          propane           propene          1_3-butadiene
##  Min.   :0.00000   Min.   :0.000000   Min.   :0.000000   Min.   :0.000000
##  1st Qu.:0.01268   1st Qu.:0.009283   1st Qu.:0.005979   1st Qu.:0.002500
##  Median :0.03547   Median :0.028409   Median :0.018482   Median :0.004167
##  Mean   :0.05042   Mean   :0.053803   Mean   :0.028772   Mean   :0.007371
##  3rd Qu.:0.07266   3rd Qu.:0.080130   3rd Qu.:0.042761   3rd Qu.:0.007500
##  Max.   :1.00000   Max.   :1.000000   Max.   :1.000000   Max.   :1.000000
##     i-butane          n-butane          acetylene        cyclopentane
##  Min.   :0.00000   Min.   :0.000000   Min.   :0.00000   Min.   :0.000000
##  1st Qu.:0.00614   1st Qu.:0.008777   1st Qu.:0.02674   1st Qu.:0.007432
##  Median :0.01925   Median :0.027522   Median :0.05135   Median :0.022668
##  Mean   :0.03837   Mean   :0.054900   Mean   :0.07436   Mean   :0.043730
##  3rd Qu.:0.05369   3rd Qu.:0.077042   3rd Qu.:0.10211   3rd Qu.:0.062653
##  Max.   :1.00000   Max.   :1.000000   Max.   :1.00000   Max.   :1.000000
##    i-pentane          n-pentane           n-hexane            isoprene
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.000000   Min.   :0.000000
##  1st Qu.:0.006303   1st Qu.:0.005681   1st Qu.:0.004703   1st Qu.:0.002801
##  Median :0.019941   Median :0.018371   Median :0.016039   Median :0.005602
##  Mean   :0.041094   Mean   :0.038859   Mean   :0.034979   Mean   :0.010315
##  3rd Qu.:0.057857   3rd Qu.:0.054837   3rd Qu.:0.049544   3rd Qu.:0.011204
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.000000   Max.   :1.000000
##    n-heptane            benzene            n-octane            toluene
##  Min.   :0.000000   Min.   :0.00000   Min.   :0.000000   Min.   :0.00000
##  1st Qu.:0.005473   1st Qu.:0.01637   1st Qu.:0.008269   1st Qu.:0.01389
##  Median :0.018348   Median :0.04222   Median :0.026009   Median :0.04276
##  Mean   :0.039328   Mean   :0.07655   Mean   :0.054341   Mean   :0.07825
##  3rd Qu.:0.055866   3rd Qu.:0.10779   3rd Qu.:0.076497   3rd Qu.:0.11333
##  Max.   :1.000000   Max.   :1.00000   Max.   :1.000000   Max.   :1.00000
##  ethyl-benzene        m&p-xylene           o-xylene
##  Min.   :0.000000   Min.   :0.000000   Min.   :0.00000
##  1st Qu.:0.007551   1st Qu.:0.007374   1st Qu.:0.00000
##  Median :0.034520   Median :0.039115   Median :0.04139
##  Mean   :0.062378   Mean   :0.077508   Mean   :0.08650
##  3rd Qu.:0.090615   3rd Qu.:0.115742   3rd Qu.:0.12881
##  Max.   :1.000000   Max.   :1.000000   Max.   :1.00000
```

- FINAL step: create matrix of processed and normalized concentrations for NMF

```r
normalized_matrix <- as.matrix(hourly_nona_bgrm_zerorepl_norm)
#important: using the normalized VOCs for this file
```

NMF section

Preprocess

Global variables

```r
components <- 4:10
```

Remove Ozone

```r
normalized_matrix_less_o3 <- normalized_matrix[ ,setdiff(colnames(normalized_matrix), "o3")]
```

Compute error matrix

```
# compute uncertainty matrix (inverse of weight?)
# Based on the Guha paper

uncertainty_matrix <- matrix(0, nrow = nrow(normalized_matrix_less_o3),
                             ncol = ncol(normalized_matrix_less_o3))
LOD_merged <- tibble(chemical = c(adjusted_background_non_voc$chemical,
                                  adjusted_background_voc$chemical),
                     LOD = c(adjusted_background_non_voc$LOD,
                             adjusted_background_voc$LOD))

LOD_merged <- tibble(chemical = names(hourly_nona_bgrm_zerorepl_norm)) %>%
  left_join(LOD_merged) %>%
  filter(chemical %in% colnames(normalized_matrix_less_o3))
```

```
## Joining with `by = join_by(chemical)`
```

```
# creating uncertainty Matrix
for (i in 1:dim(uncertainty_matrix)[1]) {
  for (j in 1:dim(uncertainty_matrix)[2]) {
    chemical <- colnames(normalized_matrix_less_o3)[j]
    xij <- normalized_matrix_less_o3[i, j]
    LOD <- LOD_merged$LOD[LOD_merged$chemical == chemical]
    # Get LOD value for this row
    if (j == 1) {
      # based on equation 6, we sqrt ch4 (at column = 1) and times by 1
      uncertainty_matrix[i, j] <- sqrt(xij)
    } else if (j == 2) {
      # 0.25 for co2
      uncertainty_matrix[i, j] <- 0.25 * sqrt(xij)
    } else if (j == 3) {
      # 0.5 for CO
      uncertainty_matrix[i, j] <- 0.5 * sqrt(xij)
    } else if (xij <= LOD) {
      uncertainty_matrix[i, j] <- 2 * LOD # equation 5a) in reference paper
    } else {
      uncertainty_matrix[i, j] <- sqrt(((0.1 * xij)**2 + LOD**2))  #equation 5c) in reference paper
    }
  }
}
```

```
# Convert zero uncertainties to the next smallest uncertainty of the corresponding compound
uncertainty_matrix[uncertainty_matrix==0]<-apply(uncertainty_matrix, 2, function(x) sort(x)[2])
```

```
## Warning in uncertainty_matrix[uncertainty_matrix == 0] <-
## apply(uncertainty_matrix, : number of items to replace is not a multiple of
## replacement length
```

```
# THIS NEEDS TO BE CHECKED IF WE WANT TO TAKE RECIPROCAL FOR EACH ELEMENT
# CURRENT RESULTS IS WHEN WEIGHT = UNCERTAINTY
# NOT POSSIBLE TO DO SIMPLY TAKE RECIPROCAL SINCE THERE'RE 0 UNCERTAINTIES
weight_matrix <- 1/uncertainty_matrix

summary(weight_matrix)
```

```
##        V1                 V2                V3                 V4
##  Min.   :  1.000   Min.   : 4.000   Min.   :  2.000   Min.   :1.250
##  1st Qu.:  5.185   1st Qu.: 8.134   1st Qu.:  8.185   1st Qu.:1.250
##  Median :  8.277   Median : 9.369   Median : 10.148   Median :1.250
##  Mean   : 10.323   Mean   : 9.623   Mean   : 10.640   Mean   :1.251
##  3rd Qu.: 13.141   3rd Qu.:10.751   3rd Qu.: 12.422   3rd Qu.:1.250
##  Max.   :491.144   Max.   :34.037   Max.   :126.797   Max.   :2.484
##        V5               V6                V7                V8
##  Min.   :1.250   Min.   : 8.944   Min.   : 9.678   Min.   : 9.746
##  1st Qu.:1.250   1st Qu.:10.000   1st Qu.:19.231   1st Qu.:21.739
##  Median :1.250   Median :10.000   Median :23.293   Median :39.121
##  Mean   :1.253   Mean   :12.384   Mean   :27.649   Mean   :33.580
##  3rd Qu.:1.250   3rd Qu.:10.000   3rd Qu.:36.985   3rd Qu.:42.365
##  Max.   :2.488   Max.   :19.900   Max.   :38.271   Max.   :43.261
##        V9               V10               V11               V12
##  Min.   : 9.859   Min.   : 9.842   Min.   : 9.903   Min.   : 9.903
##  1st Qu.:29.412   1st Qu.:27.778   1st Qu.:35.714   1st Qu.:35.714
##  Median :46.347   Median :44.285   Median :35.714   Median :54.768
##  Mean   :43.621   Mean   :40.618   Mean   :40.512   Mean   :52.185
##  3rd Qu.:56.564   3rd Qu.:54.112   3rd Qu.:35.714   3rd Qu.:68.687
##  Max.   :58.528   Max.   :55.276   Max.   :71.066   Max.   :71.074
##       V13               V14               V15               V16
##  Min.   : 9.917   Min.   : 9.187   Min.   : 9.917   Min.   : 9.95
##  1st Qu.:38.462   1st Qu.:11.628   1st Qu.:38.462   1st Qu.:50.00
##  Median :59.325   Median :21.253   Median :60.265   Median :75.75
##  Mean   :56.622   Mean   :17.687   Mean   :56.700   Mean   :73.01
##  3rd Qu.:73.720   3rd Qu.:22.820   3rd Qu.:73.711   3rd Qu.:95.52
##  Max.   :76.540   Max.   :23.140   Max.   :76.541   Max.   :99.50
##       V17              V18               V19              V20
##  Min.   : 9.95   Min.   :  9.96   Min.   : 9.94   Min.   :  9.968
##  1st Qu.:50.00   1st Qu.: 55.56   1st Qu.:45.45   1st Qu.: 62.500
##  Median :74.81   Median : 80.74   Median :45.45   Median : 89.534
##  Mean   :72.66   Mean   : 80.01   Mean   :59.24   Mean   : 89.780
##  3rd Qu.:95.23   3rd Qu.:105.43   3rd Qu.:89.08   3rd Qu.:118.592
##  Max.   :99.50   Max.   :110.56   Max.   :90.44   Max.   :124.378
##       V21               V22                V23                V24
##  Min.   :  9.96   Min.   :  9.968   Min.   :  9.968   Min.   :  9.968
##  1st Qu.: 55.56   1st Qu.: 62.500   1st Qu.: 62.500   1st Qu.: 62.500
##  Median : 85.48   Median : 91.169   Median : 88.561   Median : 81.631
##  Mean   : 80.33   Mean   : 89.312   Mean   : 86.618   Mean   : 85.245
##  3rd Qu.:105.73   3rd Qu.:119.159   3rd Qu.:118.236   3rd Qu.:114.204
##  Max.   :110.55   Max.   :124.377   Max.   :124.373   Max.   :124.279
##       V25                V26
##  Min.   :  9.968   Min.   :  9.968
##  1st Qu.: 62.500   1st Qu.: 62.500
##  Median : 69.955   Median : 62.500
##  Mean   : 80.748   Mean   : 73.996
##  3rd Qu.:111.760   3rd Qu.: 98.097
##  Max.   :124.377   Max.   :124.265
```

Helper functions for plots

```
get_fingerprint_plot <- function(H, factor_names = c('Factor 1', 'Factor 2',
                                                     'Factor 3', 'Factor 4',
```

```r
                                                    'Factor 5')){
  custom_colors <- setNames(color_pal,
                            factor_names)

  # Convert to proportions
  contrib_prop <- apply(H[,1:(length(H)-1)], MARGIN = 2,
                        FUN = function(x) {x/sum(x)})

  contrib_prop <- contrib_prop %>%
    as_tibble() %>%
    mutate(Component = factor_names) %>%
    mutate(Component = factor(Component, levels = factor_names)) %>%
    pivot_longer(cols = -Component,
                 names_to = "Chemical",
                 values_to = "Contribution_prop") %>%
    mutate(Chemical = factor(Chemical, levels = desired_order))

  return(contrib_prop %>%
    ggplot(aes(fill = Component, y = Contribution_prop, x = Chemical)) +
    geom_bar(position = "fill", stat = "identity") +
    scale_fill_manual(values = custom_colors) +
    theme(axis.text.x = element_text(angle = 45, hjust = 1)) +
    labs(x = "Chemical", y = "Contribution Proportion") +
    theme(
      panel.grid.major = element_blank(),
      panel.grid.minor = element_blank(),
      panel.background = element_blank()
    ))
}
```

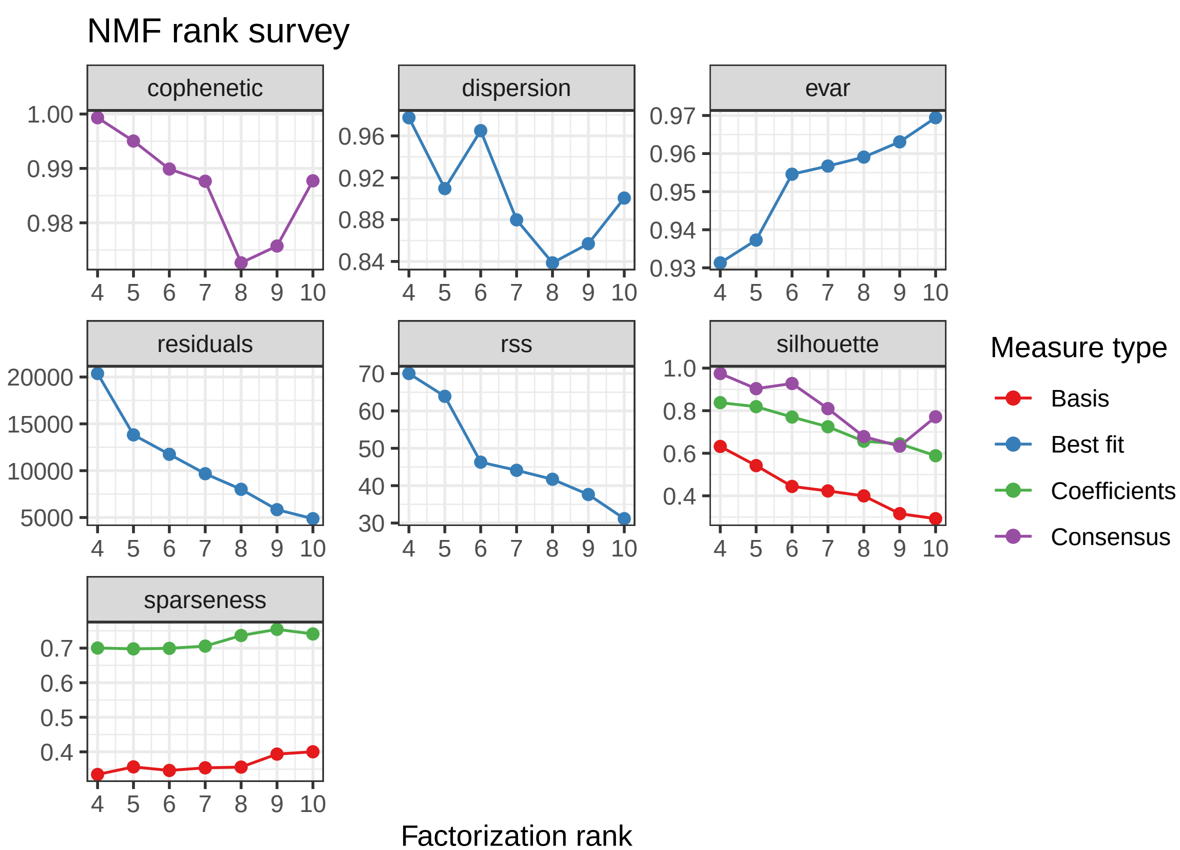
```r
hourly_wind_nona <- hourly_nona %>%
  select(wdr_deg, wsp_ms)

get_wind_plot_data <- function(W, factor_names = c('Factor 1', 'Factor 2',
                                                    'Factor 3', 'Factor 4',
                                                    'Factor 5')){

  data_to_plot <- tibble(
    component1 = W[, 1],
    component2 = W[, 2],
    component3 = W[, 3],
    component4 = W[, 4],
    component5 = W[, 5],
    wd = round(hourly_wind_nona$wdr_deg, -1)
  )

  data_long <- data_to_plot %>%
  pivot_longer(cols = starts_with("component"), names_to = "Factor", values_to = "Expression")

  data_long <- data_long %>%
    mutate(wd = factor(wd, levels = sort(unique(wd))))

  data_long
}
```

```r
get_wind_plots <- function(W, y_axis_upper = rep(10, 5),
                                factor_names = c('Factor 1', 'Factor 2',
                                                 'Factor 3', 'Factor 4',
                                                 'Factor 5')){
  data_long <- get_wind_plot_data(W, factor_names)

  # Select every second wind direction for labeling
  every_second_label <- levels(data_long$wd)[seq(1, length(levels(data_long$wd)), by = 2)]

  factor_labels <- setNames(paste(c('Factor 1', 'Factor 2','Factor 3', 'Factor 4',
                                    'Factor 5'), ' - ', factor_names), paste0('component', 1:5))

  y_axis_limits <- list(
    "component1" = c(0, y_axis_upper[1]),
    "component2" = c(0, y_axis_upper[2]),
    "component3" = c(0, y_axis_upper[3]),
    "component4" = c(0, y_axis_upper[4]),
    "component5" = c(0, y_axis_upper[5])
  )


  plots <- lapply(1:5, function(i) {
    factor_name <- paste0("component", i)

    ggplot(data_long %>% filter(Factor == factor_name),
           aes(x = wd, y = Expression, fill = as.factor(wd))) +
      geom_boxplot(outliers=F, size=0.3) +
      scale_fill_manual(values = rep(color_pal[i], length(unique(data_long$wd)))) +
      scale_x_discrete(breaks = every_second_label) +
      coord_cartesian(ylim = y_axis_limits[[factor_name]]) +
      scale_y_continuous(
        limits = c(0, NA),
        breaks = seq(0, y_axis_limits[[factor_name]][2], length.out = 5) ,
        expand=expansion(mult=c(0))
      ) +
      labs(title = factor_labels[factor_name],
           x = "Wind Direction (°)",
           y = "Factor Expression") +
      theme_minimal() +
      theme(
        legend.position = "none",
        plot.title = element_text(size = 6),  # Smaller title text
        axis.title = element_text(size = 6),  # Smaller axis labels
        axis.text = element_text(size = 6),  # Smaller x and y tick labels
        axis.text.x = element_text(angle = 45, hjust = 1)
      )
  })

  return(plots)
}
```

LS-NMF + Random seed

```r
# for each rank, run 30 models and find best one
# start_time_lsnmf_rand <- Sys.time()
#
# lsnmf_random_less_o3 <- nmf(
#   normalized_matrix_less_o3,
#   components,
#   method = "ls-nmf",
#   weight = weight_matrix,
#   30,
#   seed = 123456
# )
#
# end_time_lsnmf_rand <- Sys.time()
# end_time_lsnmf_rand-start_time_lsnmf_rand
# # 19.25 minutes to run the above

# saveRDS(lsnmf_random_less_o3,
#         'lsnmf_random_less_o3.rds')
lsnmf_random_less_o3 <- readRDS('lsnmf_random_less_o3.rds')
```

```r
# plots the NMF rank survey
plot(lsnmf_random_less_o3)
```



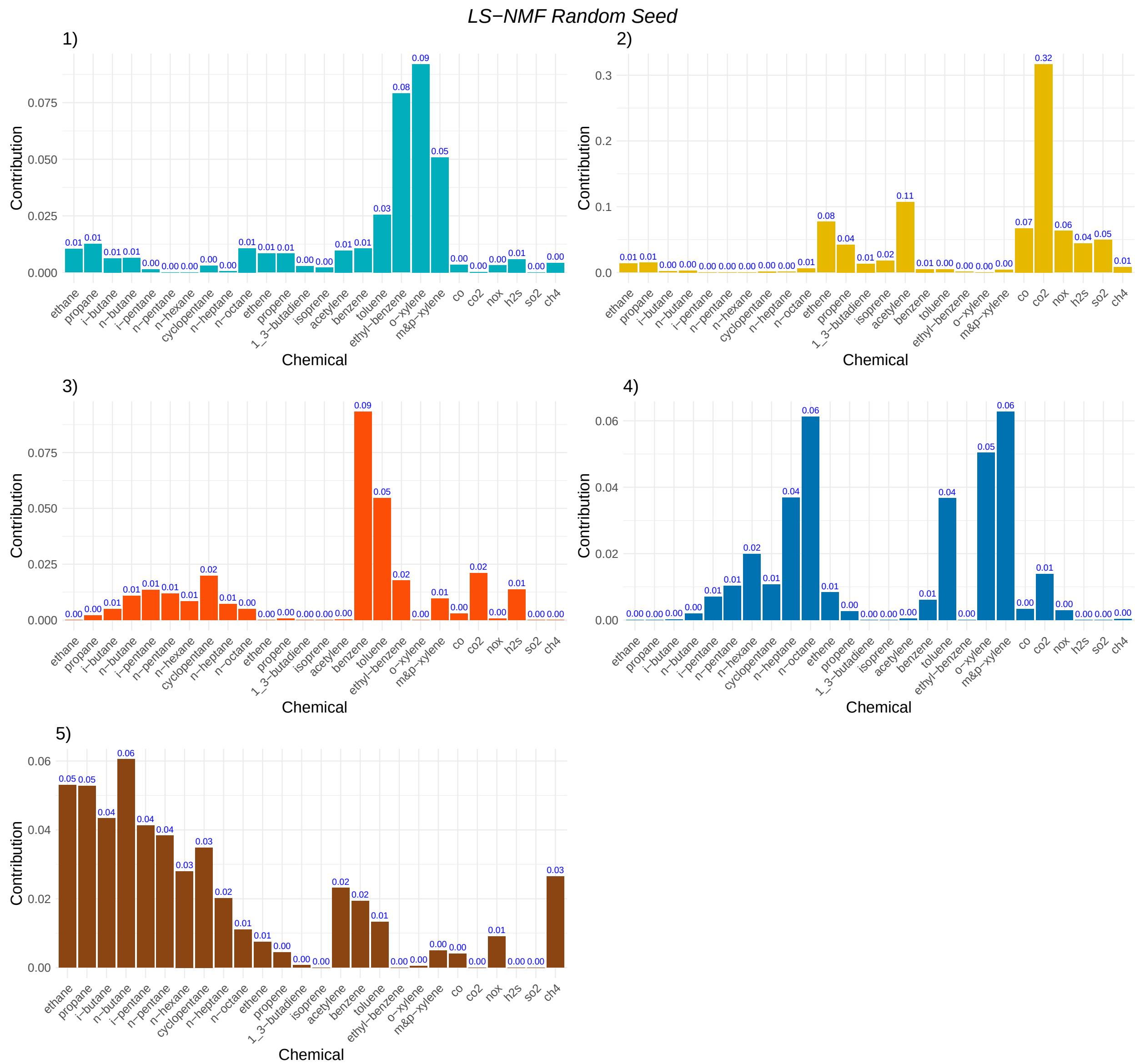
Look at 5 factors:

```
output <- lsnmf_random_less_o3$fit$`5`
W <- basis(output)
H <- coef(output)
```

Source Contribution plots

- Source Contribution plots

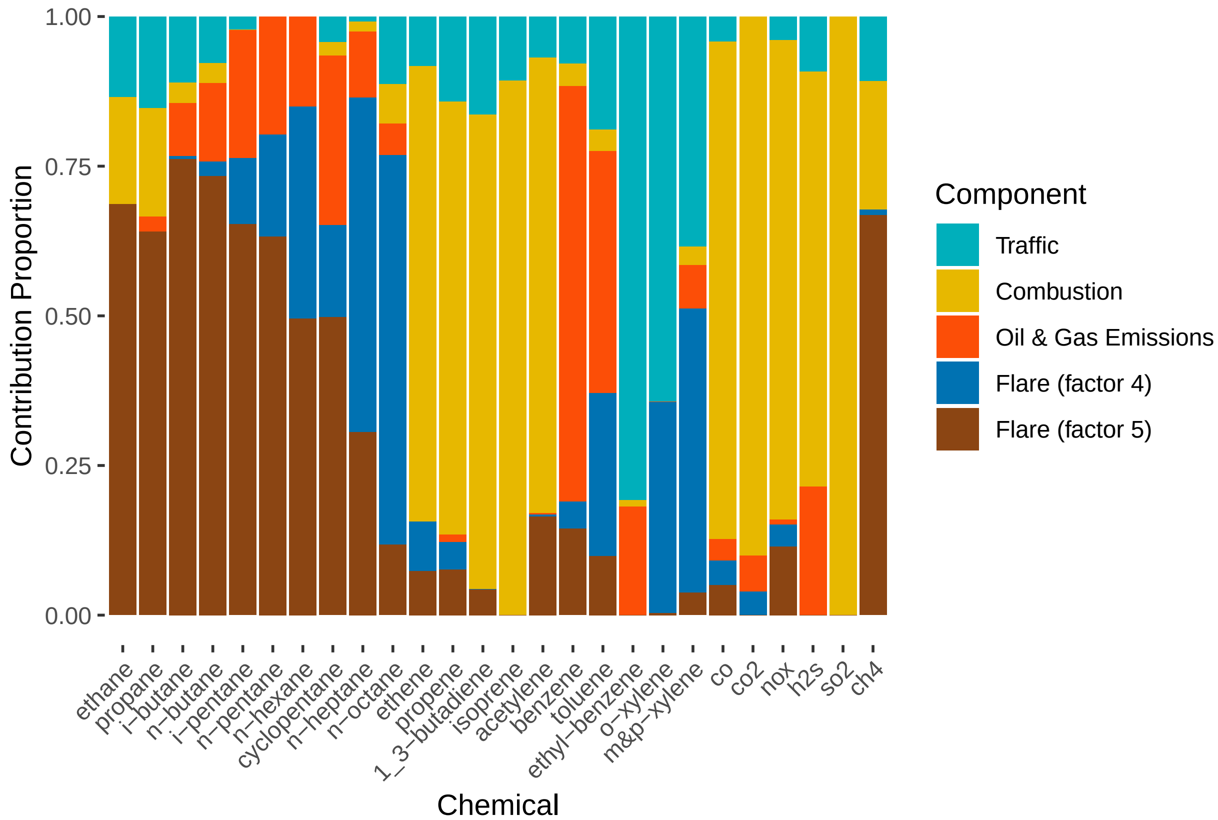
```
# Convert H to a data frame for ggplot
H_df_5c_less_o3 <- as.data.frame(H)
# Add a column for chemicals
H_df_5c_less_o3$Component <- rownames(H_df_5c_less_o3)

# Reshape data to long format
H_long_5c_less_o3 <- pivot_longer(H_df_5c_less_o3, cols = -Component,
                                  names_to = "Chemical", values_to = "Contribution")

# Plot
nmfplt_1_lsnmf_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                           '1', '1)')
nmfplt_2_lsnmf_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                           '2', '2)')
nmfplt_3_lsnmf_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                           '3', '3)')
nmfplt_4_lsnmf_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                           '4', '4)')
nmfplt_5_lsnmf_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                           '5', '5)')
```



Fingerprint plot

- Fingerprint plots

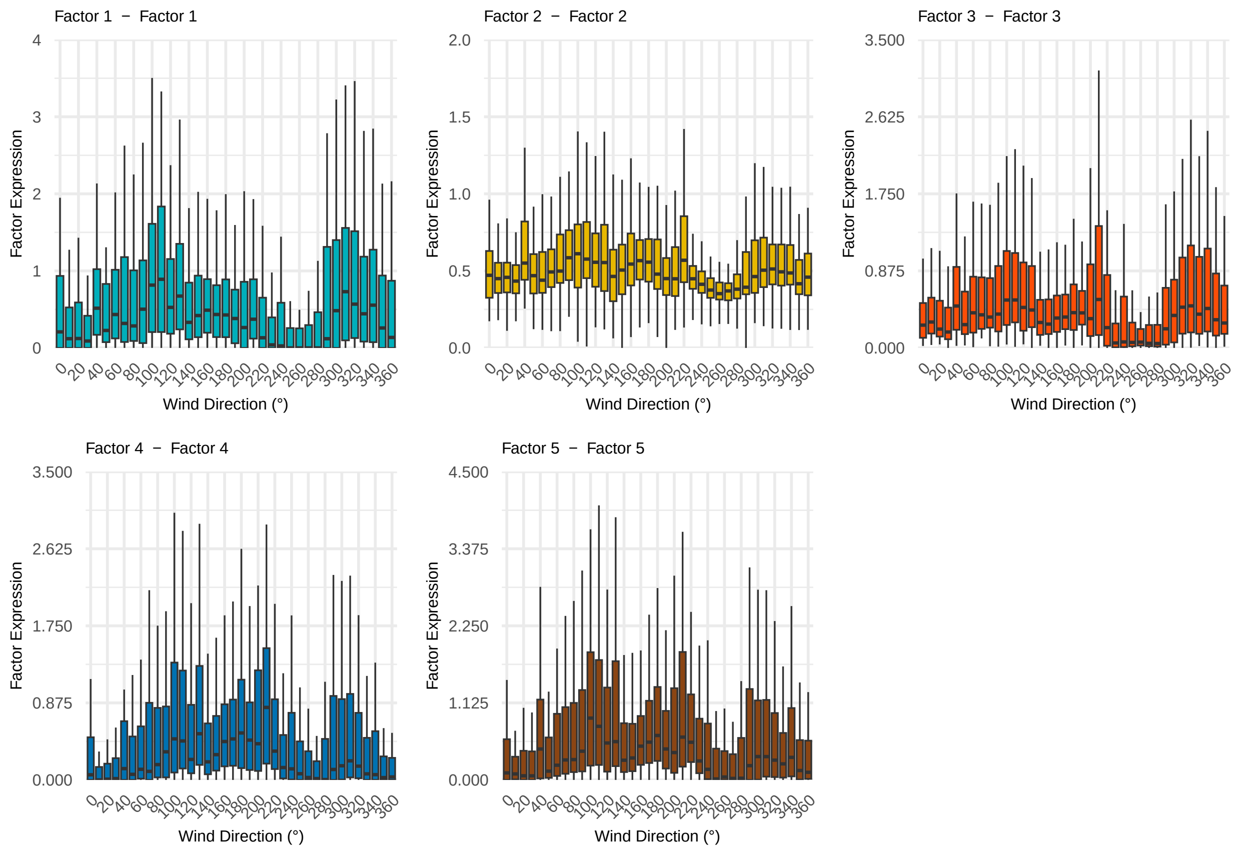
```
fingerprint <- get_fingerprint_plot(H_df_5c_less_o3, c(
      'Traffic',
      'Combustion',
      'Oil & Gas Emissions',
      'Flare (factor 4)',
      'Flare (factor 5)'
    ))

fingerprint
```



Wind plot

- Wind plots

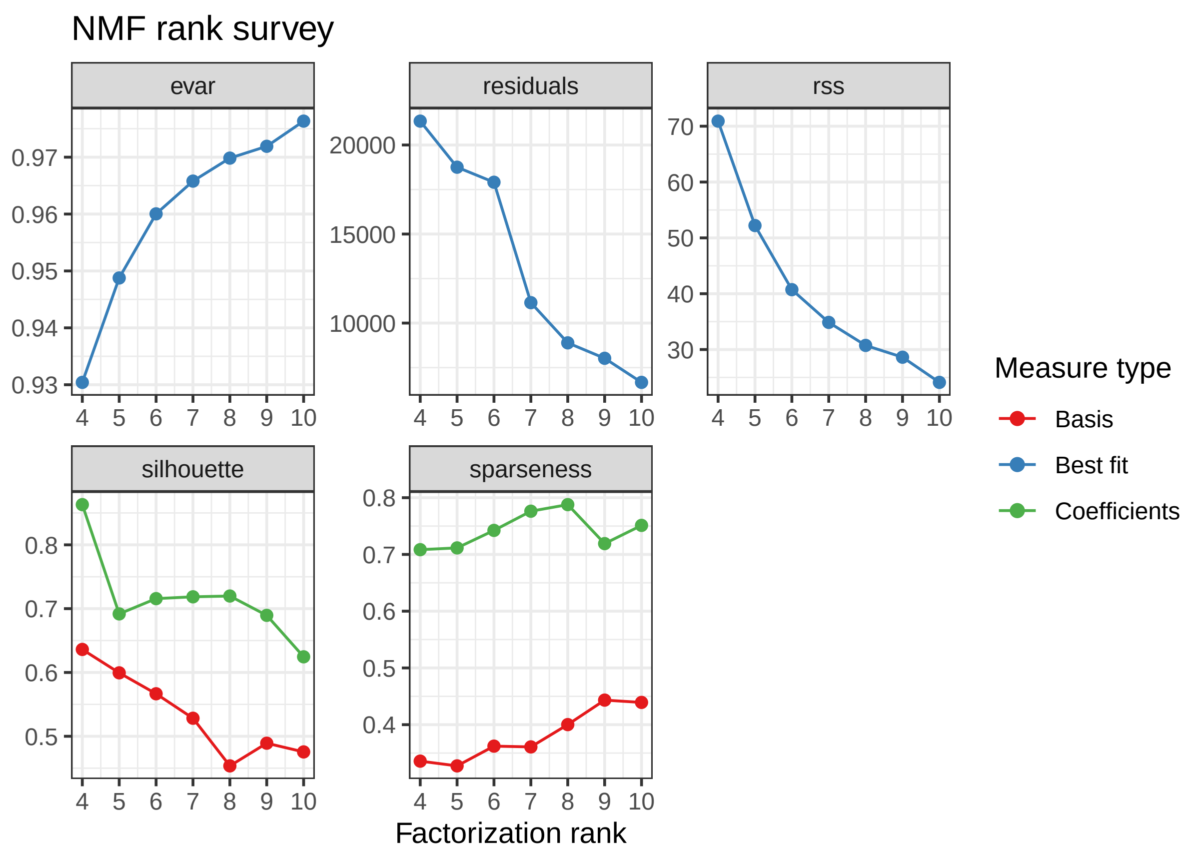
```
wind_plot <- get_wind_plots(W, y_axis_upper = c(4, 2, 3.5, 3.5, 4.5))

grid.arrange(grobs = wind_plot, ncol = 3)
```



LS-NMF + nndsvd seed

```r
# Run nmf with 4:10 components and nndsvd seed
# start_time_lsnmf_nndsvd <- Sys.time()
#
# lsnmf_nndsvd_less_o3 <- nmf(
#   normalized_matrix_less_o3,
#   rank = components,
#   nrun = 1, # since using nndsvd
#   method = "ls-nmf",
#   weight = weight_matrix,
#   seed = 'nndsvd'
# )
#
# end_time_lsnmf_nndsvd <- Sys.time()
# end_time_lsnmf_nndsvd-start_time_lsnmf_nndsvd
# # # 1.34 minutes to run the above
# #
# saveRDS(lsnmf_nndsvd_less_o3,
#         'lsnmf_nndsvd_less_o3.rds')

lsnmf_nndsvd_less_o3 <- readRDS('lsnmf_nndsvd_less_o3.rds')
```

```r
# plots the NMF rank survey
plot(lsnmf_nndsvd_less_o3)
```



Look at 5 factors:

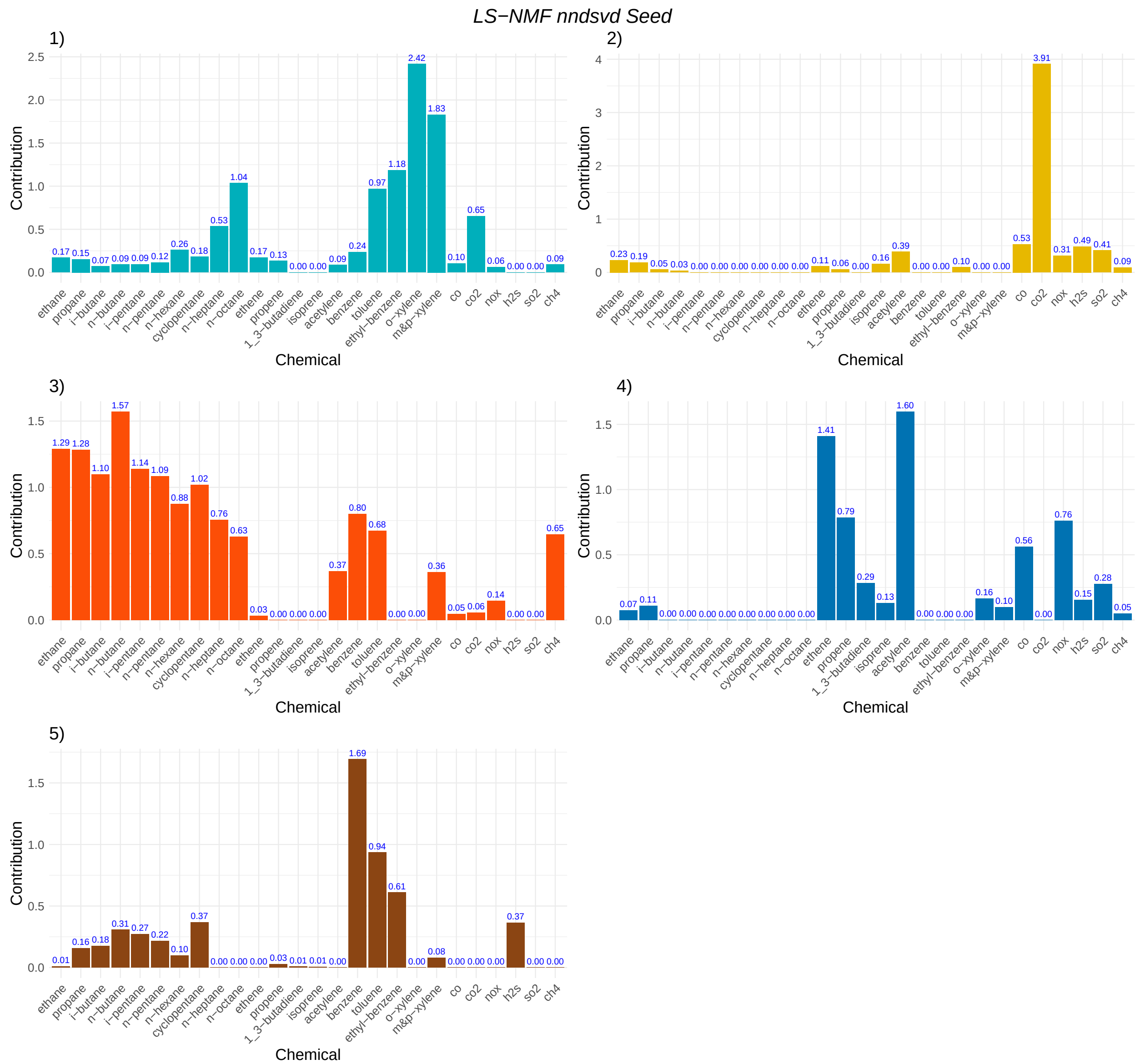
```
output <- lsnmf_nndsvd_less_o3$fit$`5`
W <- basis(output)
H <- coef(output)
```

Source Contribution plots

- Source Contribution plots

```
# Convert H to a data frame for ggplot
H_df_5c_less_o3 <- as.data.frame(H)
# Add a column for chemicals
H_df_5c_less_o3$Component <- rownames(H_df_5c_less_o3)

# Reshape data to long format
H_long_5c_less_o3 <- pivot_longer(H_df_5c_less_o3, cols = -Component,
                                   names_to = "Chemical", values_to = "Contribution")

# Plot
nmfplt_1_lsnmf_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '1', '1)')
nmfplt_2_lsnmf_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '2', '2)')
nmfplt_3_lsnmf_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '3', '3)')
```

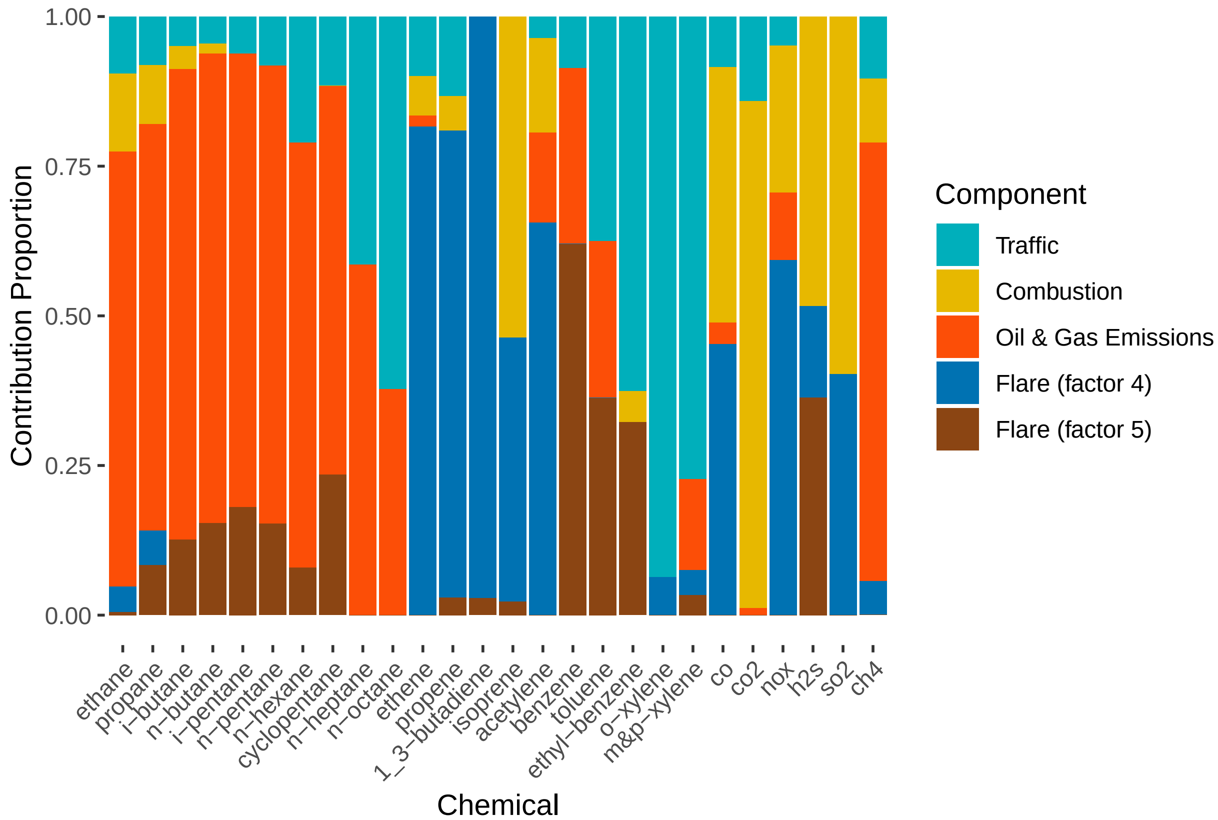
```r
nmfplt_4_lsnmf_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                        '4', '4)')
nmfplt_5_lsnmf_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                        '5', '5)')
```



Fingerprint plot

- Fingerprint plots

```r
fingerprint <- get_fingerprint_plot(H_df_5c_less_o3, c(
      'Traffic',
      'Combustion',
      'Oil & Gas Emissions',
      'Flare (factor 4)',
      'Flare (factor 5)'
    ))
fingerprint
```

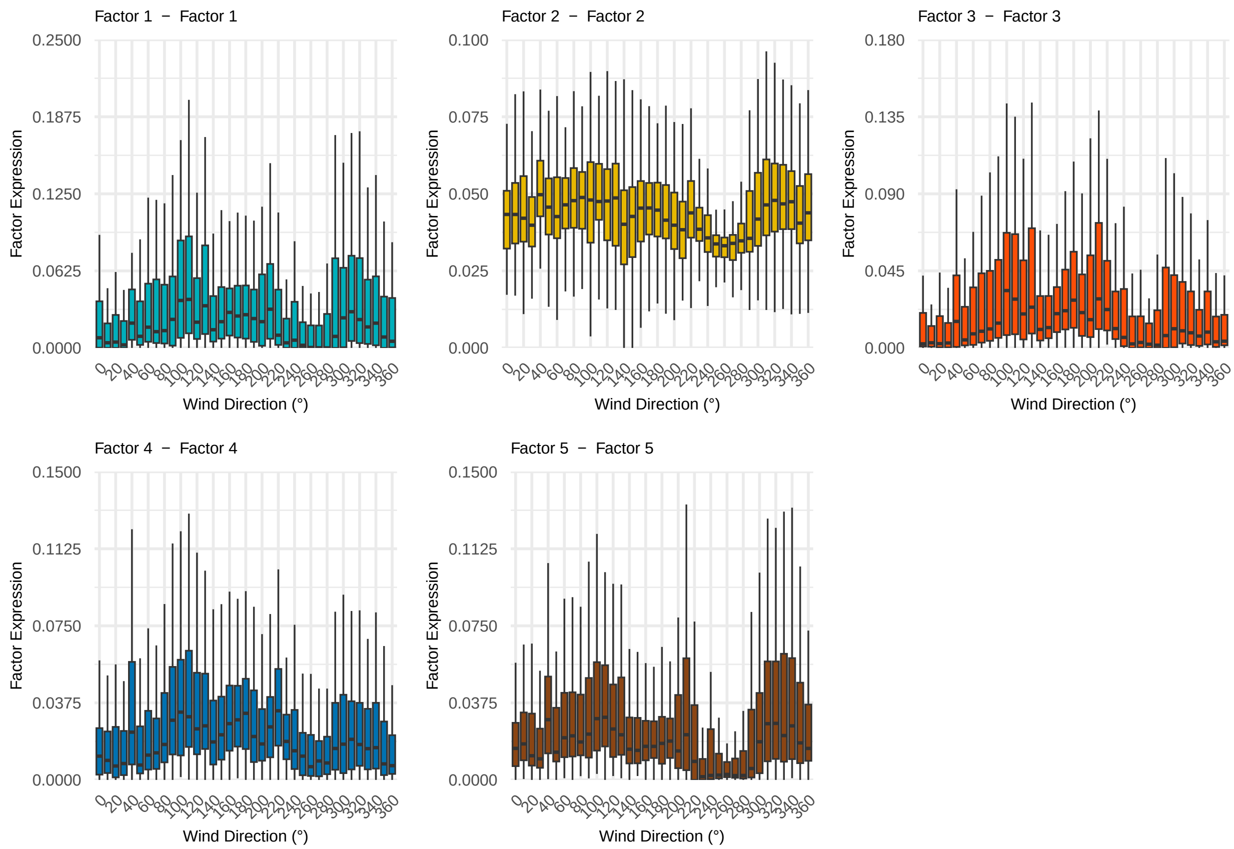



```
#ggsave("fingerprint.png", c)
```

Wind plot

- Wind plots

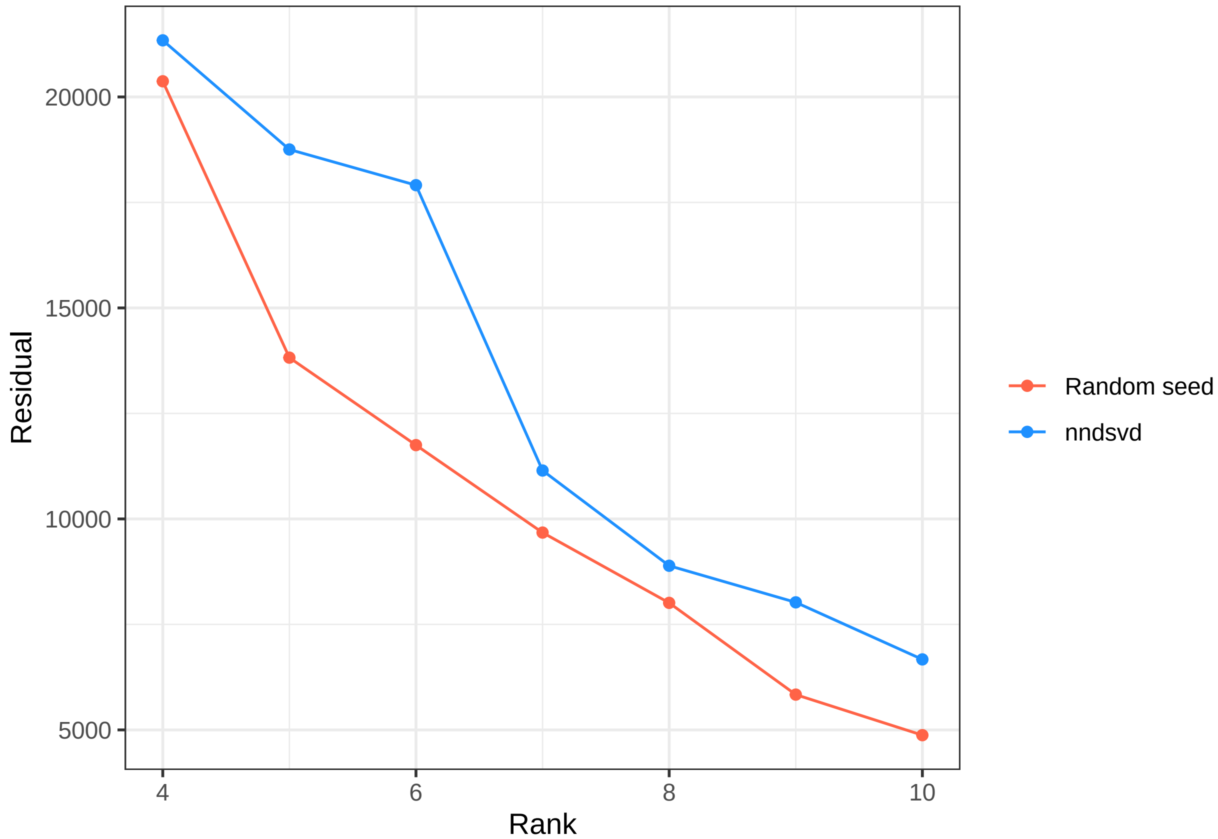
```
wind_plot <- get_wind_plots(W, y_axis_upper = c(0.25, 0.1, 0.18, 0.15, 0.15))
grid.arrange(grobs = wind_plot, ncol = 3)
```



Comparing random seed vs nndsvd for ls-nmf

Residuals is defined as sum(((X - fitted(object)) * weight)^2)/2

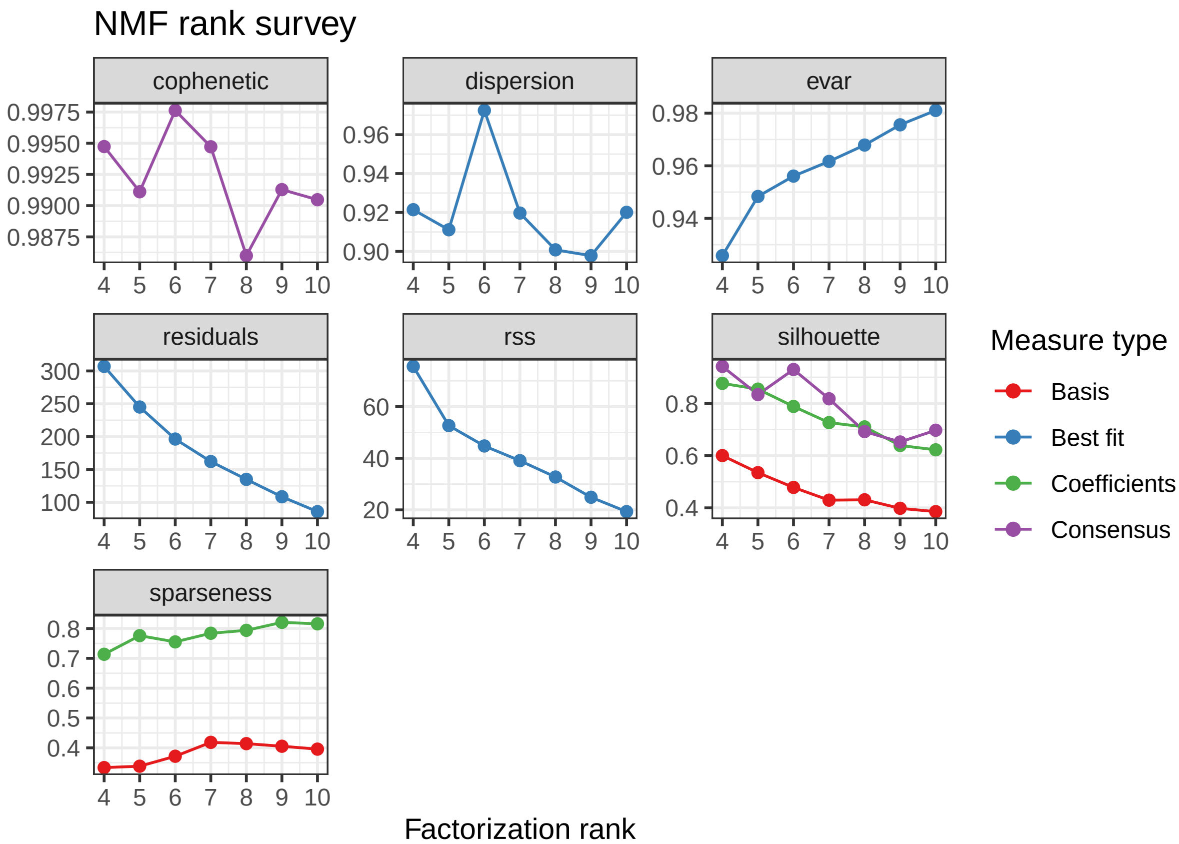
```
tibble(component = components,
       random_residual = lsnmf_random_less_o3$measures$residuals,
       nndsvd_residual = lsnmf_nndsvd_less_o3$measures$residuals) %>%
  ggplot() +
  geom_line(aes(x = component, y =random_residual, color = 'Random seed')) +
  geom_point(aes(x = component, y =random_residual, color = 'Random seed')) +
  geom_line(aes(x = component, y = nndsvd_residual, color = 'nndsvd')) +
  geom_point(aes(x = component, y = nndsvd_residual, color = 'nndsvd')) +
  scale_colour_manual("",
                      breaks = c("Random seed", "nndsvd"),
                      values = c("tomato1", "dodgerblue")) +
  labs(x = 'Rank', y = 'Residual', 'WRSS') +
  theme_bw()
```



KL + Random seed

```
# start_time_kl_random <- Sys.time()
#
# kl_random_less_o3 <- nmf(
#   normalized_matrix_less_o3,
#   rank = components,
#   nrun = 30,
#   method = "KL",
#   seed = 123456
# )
#
# end_time_kl_random <- Sys.time()
# end_time_kl_random-start_time_kl_random
# 14.27 minutes to run the above

# saveRDS(kl_random_less_o3, 'kl_random_less_o3.rds')

kl_random_less_o3 <- readRDS('kl_random_less_o3.rds')
```

```
# plots the NMF rank survey
plot(kl_random_less_o3)
```



Look at 5 factors:

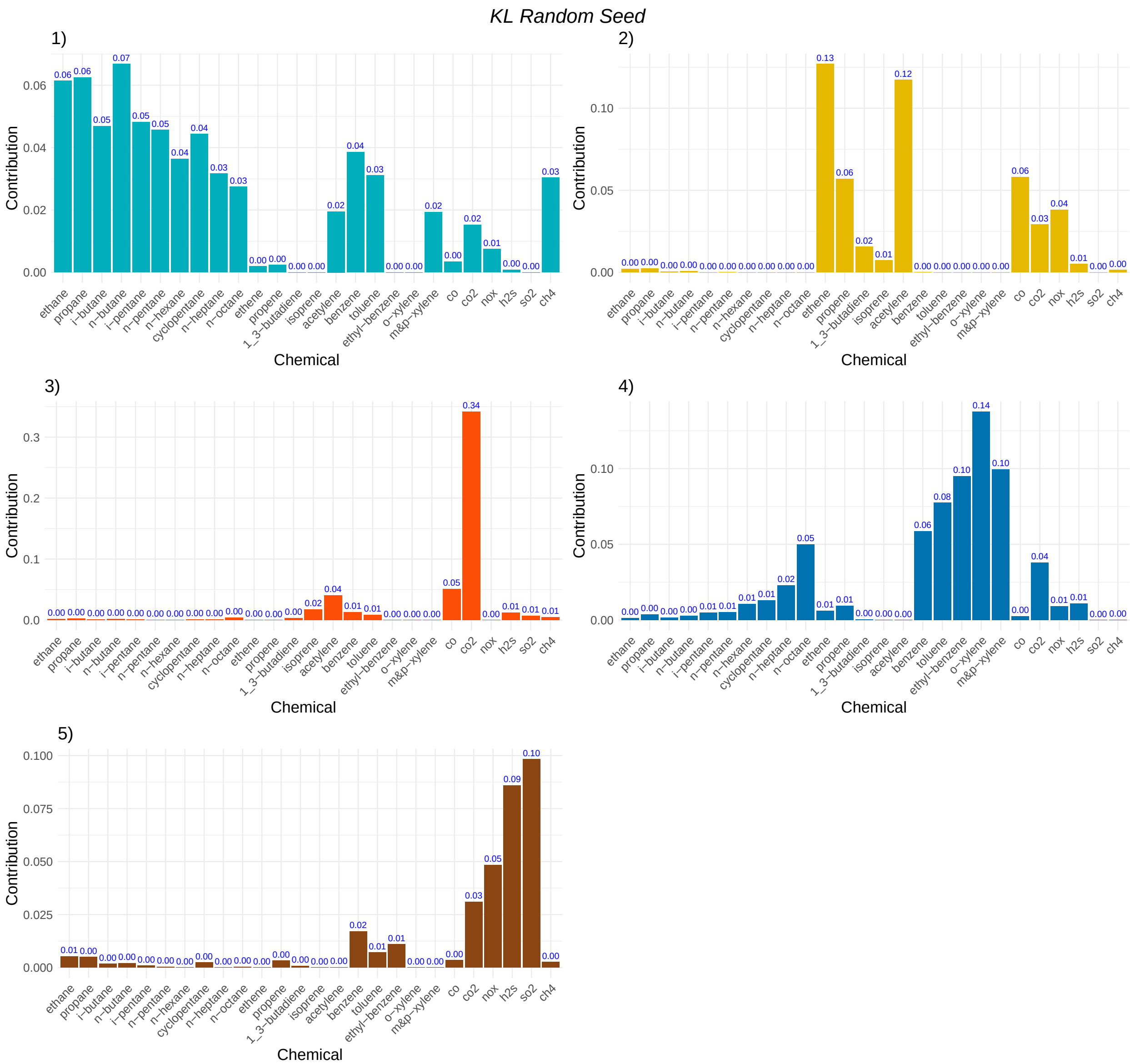
```
output <- kl_random_less_o3$fit$`5`
W <- basis(output)
H <- coef(output)
```

Source Contribution plots

- Source Contribution plots

```
# Convert H to a data frame for ggplot
H_df_5c_less_o3 <- as.data.frame(H)
# Add a column for chemicals
H_df_5c_less_o3$Component <- rownames(H_df_5c_less_o3)

# Reshape data to long format
H_long_5c_less_o3 <- pivot_longer(H_df_5c_less_o3, cols = -Component,
                                  names_to = "Chemical", values_to = "Contribution")

# Plot
nmfplt_1_kl_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                    '1', '1)')
nmfplt_2_kl_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                    '2', '2)')
nmfplt_3_kl_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                    '3', '3)')
```

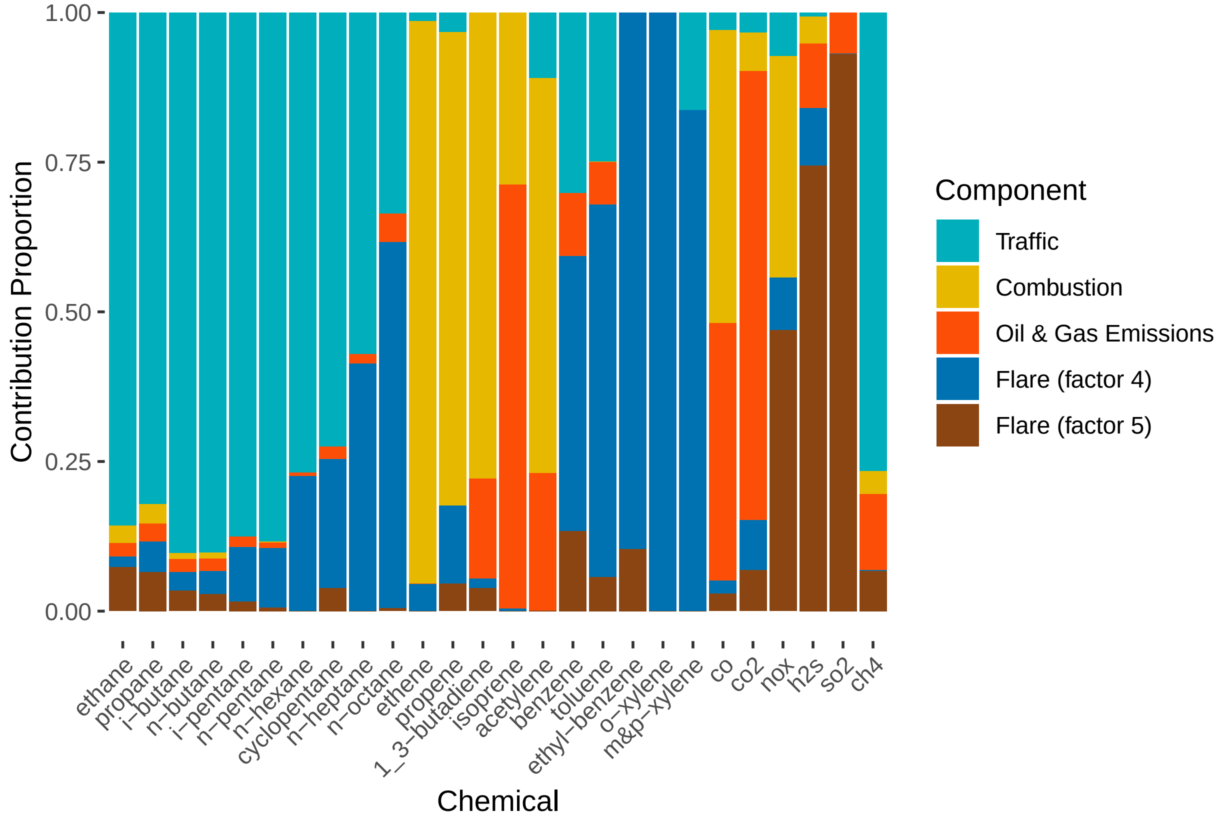
```r
nmfplt_4_kl_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                    '4', '4)')
nmfplt_5_kl_random_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                                    '5', '5)')
```



Fingerprint plot

- Fingerprint plots

```r
fingerprint <- get_fingerprint_plot(H_df_5c_less_o3, c(
      'Traffic',
      'Combustion',
      'Oil & Gas Emissions',
      'Flare (factor 4)',
      'Flare (factor 5)'
    ))
fingerprint
```

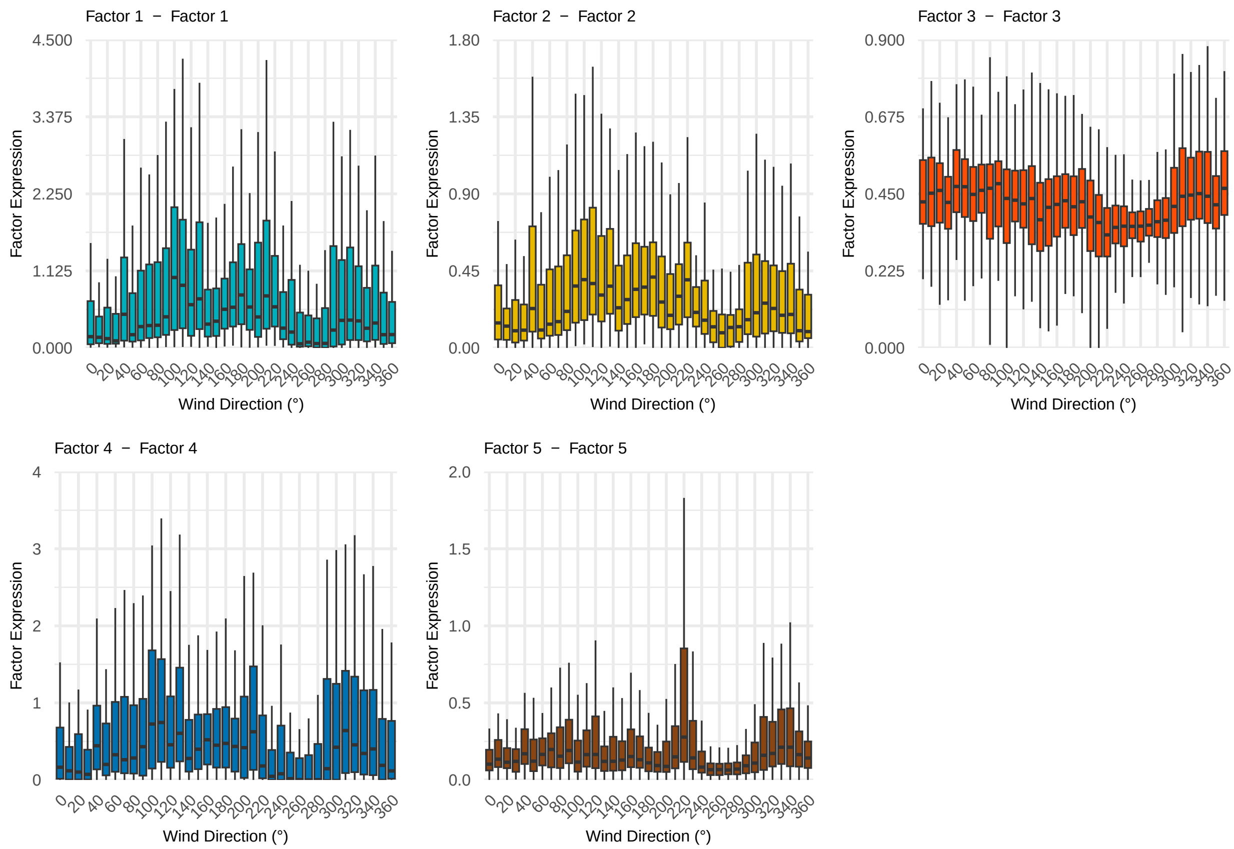



```
#ggsave("fingerprint.png", c)
```

Wind plot

- Wind plots

```
wind_plot <- get_wind_plots(W, y_axis_upper = c(4.5, 1.8, 0.9, 4, 2))
grid.arrange(grobs = wind_plot, ncol = 3)
```

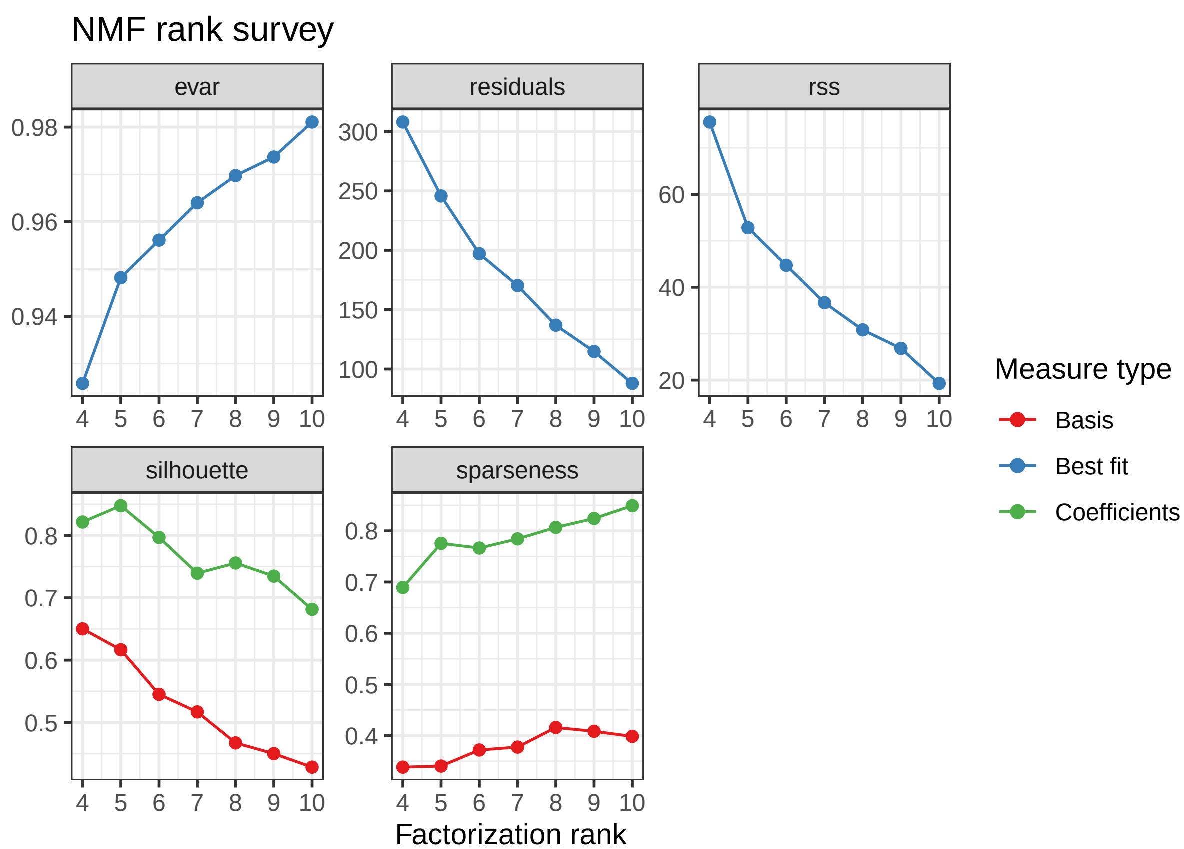


KL + nndsvd

```
# errors <- numeric(length(components) - 4)

# Loop over the number of components
# for (n in components) {
#   nmf_result <- nmf(normalized_matrix_less_o3, rank = n, method = "KL", seed='nndsvd')
#   reconstruction <- basis(nmf_result) %*% coef(nmf_result)
#   error <- norm(normalized_matrix_less_o3 - reconstruction, type = "F")^2 # RSS
#   errors[n-3] <- error
#   print(paste0('Completed ', n - 3, ' out of 7'))
# }
#
# saveRDS(errors, 'errors_KL_nndsvd_less_o3.rds')
#
# errors <- readRDS('errors_KL_nndsvd_less_o3.rds')

# start_time_kl_nndsvd <- Sys.time()
#
# kl_nndsvd_less_o3 <- nmf(
#   normalized_matrix_less_o3,
#   rank = components,
#   nrun = 1,
#   method = "KL",
#   seed = 'nndsvd'
```

```
# )
#
# end_time_kl_nndsvd <- Sys.time()
# end_time_kl_nndsvd-start_time_kl_nndsvd
# 1 minute to run the above

# saveRDS(kl_nndsvd_less_o3, 'kl_nndsvd_less_o3.rds')

kl_nndsvd_less_o3 <- readRDS('kl_nndsvd_less_o3.rds')
```

```
# plots the NMF rank survey
plot(kl_nndsvd_less_o3)
```



Look at 5 factors:

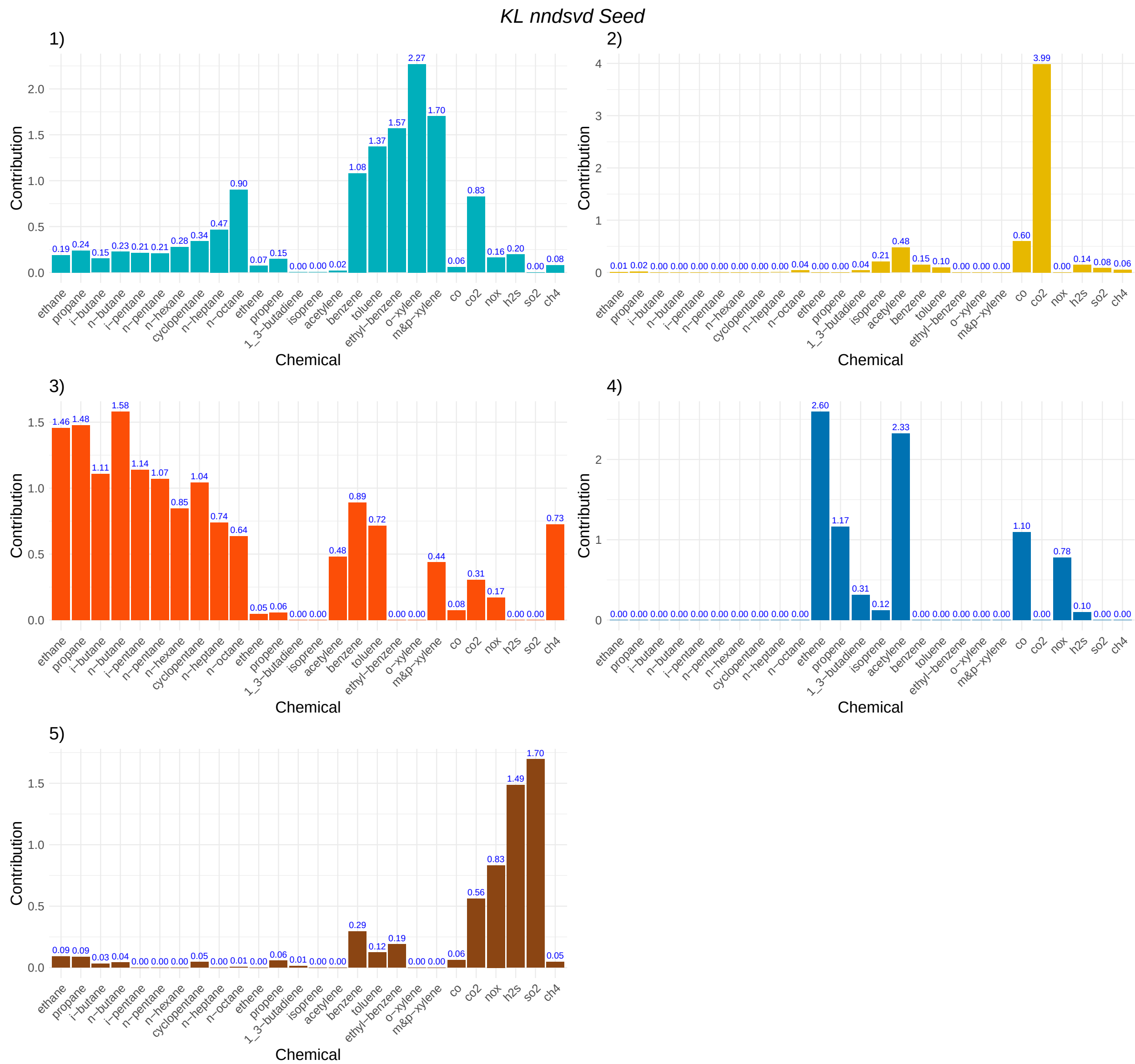
```
output <- kl_nndsvd_less_o3$fit$`5`
W <- basis(output)
H <- coef(output)
```

Source Contribution plots

- Source Contribution plots

```
# Convert H to a data frame for ggplot
H_df_5c_less_o3 <- as.data.frame(H)
# Add a column for chemicals
```

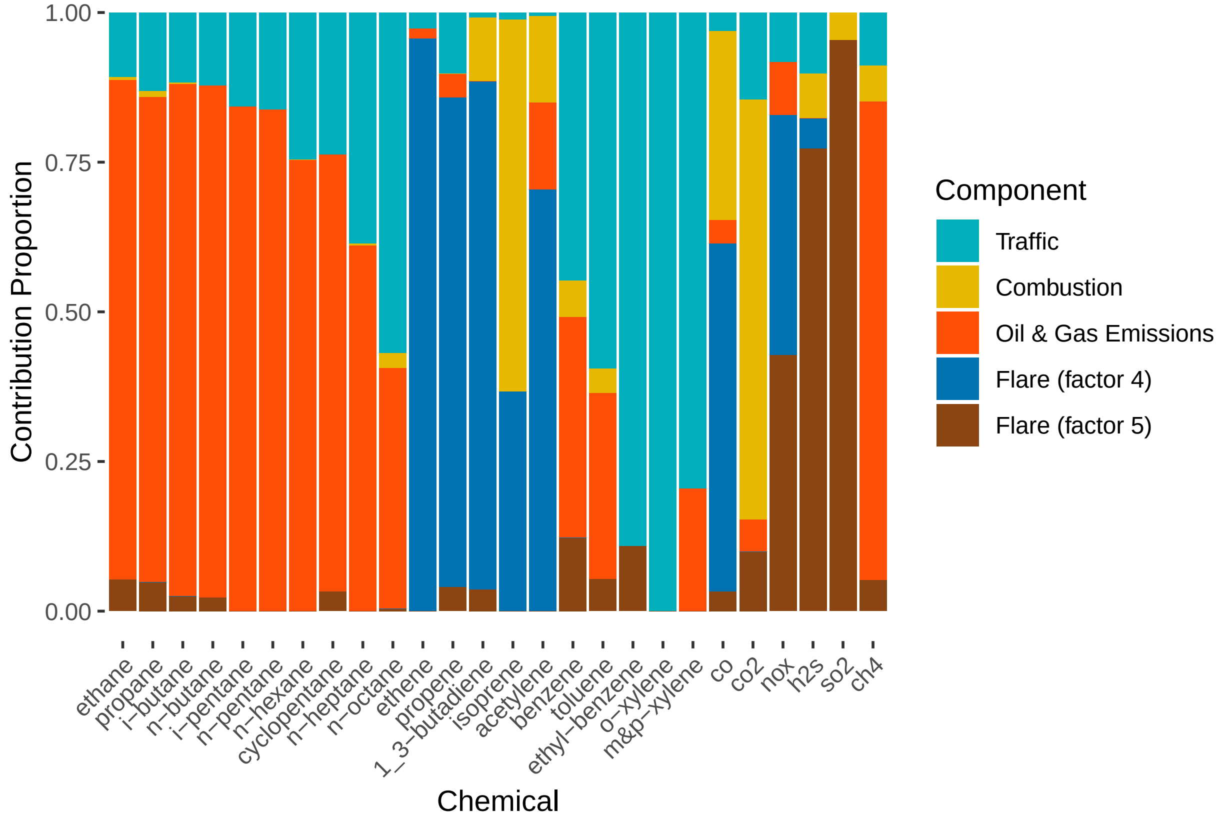
```r
H_df_5c_less_o3$Component <- rownames(H_df_5c_less_o3)

# Reshape data to long format
H_long_5c_less_o3 <- pivot_longer(H_df_5c_less_o3, cols = -Component,
                                  names_to = "Chemical", values_to = "Contribution")

# Plot
nmfplt_1_kl_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '1', '1)')
nmfplt_2_kl_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '2', '2)')
nmfplt_3_kl_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '3', '3)')
nmfplt_4_kl_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '4', '4)')
nmfplt_5_kl_nndsvd_less_o3_5c <- get_component_plot(H_long_5c_less_o3,
                                            '5', '5)')
```



Fingerprint plot

- Fingerprint plots

```
fingerprint <- get_fingerprint_plot(H_df_5c_less_o3, c(
      'Traffic',
      'Combustion',
      'Oil & Gas Emissions',
      'Flare (factor 4)',
      'Flare (factor 5)'
    ))
fingerprint
```

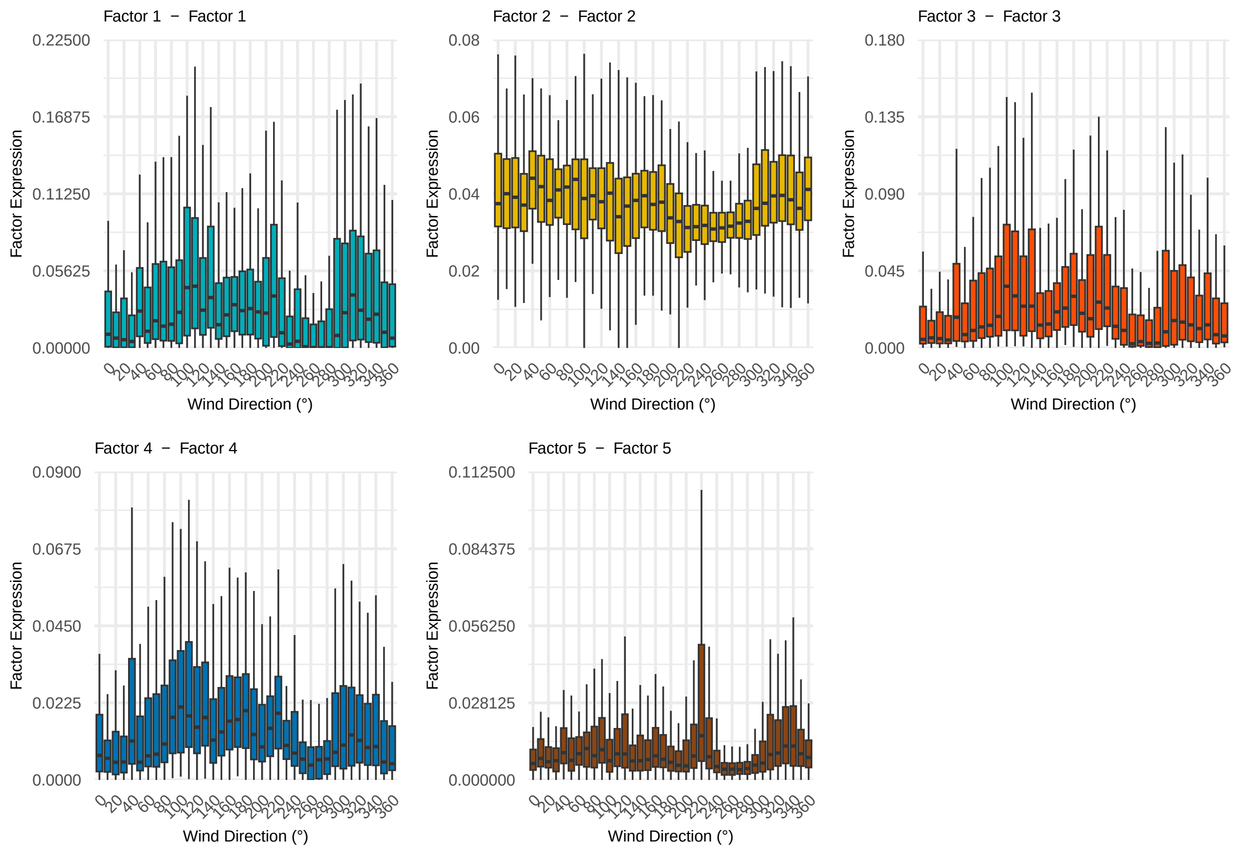



```r
#ggsave("fingerprint.png", c)
```

Wind plot

- Wind plots

```r
wind_plot <- get_wind_plots(W, y_axis_upper = c(0.225, 0.08, 0.18, 0.09, 0.1125))
grid.arrange(grobs = wind_plot, ncol = 3)
```

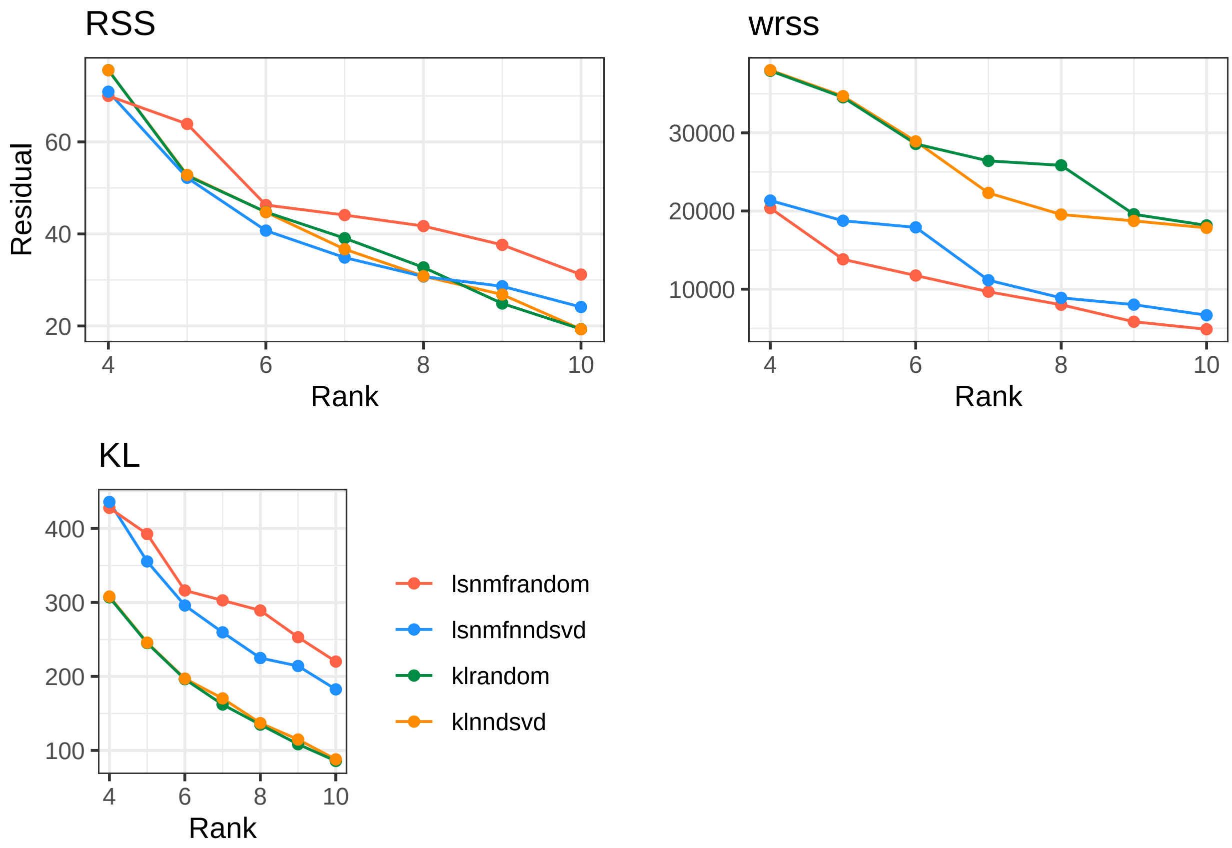


Comparing all four methods

Using RSS, WRSS, and KL

```
get_residual <- function(component, seed, method, objective) {
  fitted <- fitted(get(paste(method, seed, 'less_o3', sep = '_'))$fit[[component-3]])
  if (objective == 'wrss') {
    return(sum(((normalized_matrix_less_o3 - fitted) * weight_matrix)^2)/2)
  } else if (objective == 'kl') {
    log_term <- normalized_matrix_less_o3/fitted
    log_term[log_term<.Machine$double.eps] <- .Machine$double.eps
    return(sum(normalized_matrix_less_o3 * log(log_term) + fitted - normalized_matrix_less_o3))
  } else if (objective == 'rss') {
    return(norm(normalized_matrix_less_o3 - fitted, type = 'F')^2)
  }
}

df_plot <- expand_grid(
  component = components,
  seed = c('random', 'nndsvd'),
  method = c('lsnmf', 'kl'),
  objective = c('rss', 'wrss', 'kl')
) %>%
  rowwise() %>%
  mutate(residual = get_residual(component, seed, method, objective)) %>%
  ungroup() %>%
```

```
  mutate(model = paste0(method, seed))

RSS_plot <- df_plot %>%
  filter(objective=='rss') %>%
  ggplot() +
  geom_line(aes(x = component, y = residual, group = model, color = model)) +
  geom_point(aes(x = component, y = residual, group = model, color = model)) +
  scale_colour_manual("",
                      breaks = c("lsnmfrandom", "lsnmfnndsvd",
                                 "klrandom", "klnndsvd"),
                      values = c("tomato1", "dodgerblue",
                                 "springgreen4", "darkorange")) +
  labs(x = 'Rank', y = 'Residual', title = 'RSS') +
  theme_bw() +
  theme(legend.position="none")

WRSS_plot <- df_plot %>%
  filter(objective=='wrss') %>%
  ggplot() +
  geom_line(aes(x = component, y = residual, group = model, color = model)) +
  geom_point(aes(x = component, y = residual, group = model, color = model)) +
  scale_colour_manual("",
                    breaks = c("lsnmfrandom", "lsnmfnndsvd",
                               "klrandom", "klnndsvd"),
                    values = c("tomato1", "dodgerblue",
                               "springgreen4", "darkorange")) +
  labs(x = 'Rank', y = '', title = 'wrss') +
  theme_bw() +
  theme(legend.position="none")

KL_plot <- df_plot %>%
  filter(objective=='kl') %>%
  ggplot() +
  geom_line(aes(x = component, y = residual, group = model, color = model)) +
  geom_point(aes(x = component, y = residual, group = model, color = model)) +
  scale_colour_manual("",
                      breaks = c("lsnmfrandom", "lsnmfnndsvd",
                                 "klrandom", "klnndsvd"),
                      values = c("tomato1", "dodgerblue",
                                 "springgreen4", "darkorange")) +
  labs(x = 'Rank', y = '', title = 'KL') +
  theme_bw()
grid.arrange(RSS_plot, WRSS_plot, KL_plot, ncol=2)
```



NMF with 5 source factors without ozone

- remove ozone
- use KL divergence loss with svd seed
- Extract W (basis) and H (coefs) matrices
- Calculate variance explained in all 5 factors
- Calculate variance explained by each factor

```
nmf_result_5c_less_o3 <- kl_nndsvd_less_o3$fit$`5`

basis_matrix_5c_less_o3 <- basis(nmf_result_5c_less_o3) #W
coef_matrix_5c_less_o3 <- coef(nmf_result_5c_less_o3) #H

# get variance explained by the factors (total residuals)
reconstruct<-fitted(nmf_result_5c_less_o3)

tss <- sum((normalized_matrix_less_o3 - mean(normalized_matrix_less_o3))^2)
rss <- sum((normalized_matrix_less_o3 - reconstruct)^2)
variance_explained <- 1 - (rss / tss)
variance_explained
```

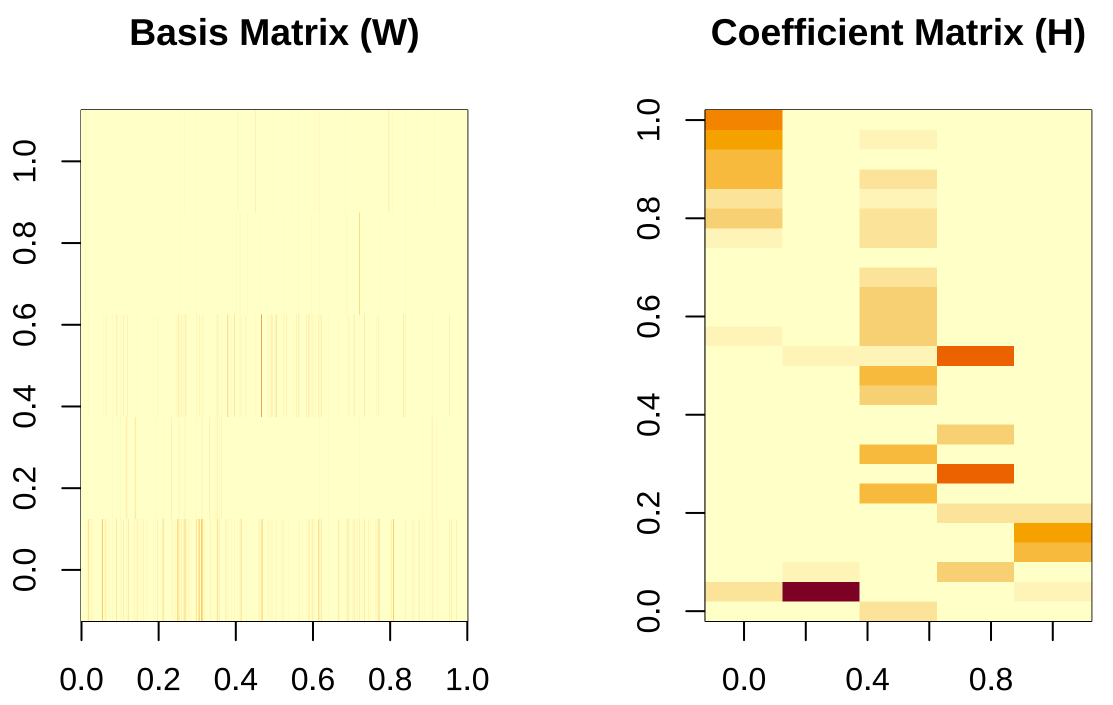
```
## [1] 0.9212864
```

```
# get variance explained by each factor separately
# Compute variance explained by each factor
# Initialize variance explained tracker
variance_explained_factors <- numeric(5)
```

```r
# Incrementally add factors and calculate variance explained
reconstruction <- matrix(0, nrow = nrow(basis_matrix_5c_less_o3), ncol = ncol(coef_matrix_5c_less_o3))

for (i in 1:5) {
  # Add the i-th factor to the reconstruction
  reconstruction <- reconstruction + (basis_matrix_5c_less_o3[, i, drop=FALSE] %*% coef_matrix_5c_less_

  # Compute Residual Sum of Squares (RSS)
  rss_f <- sum((normalized_matrix_less_o3 - reconstruction)^2)

  # Compute Variance Explained by adding this factor
  variance_explained_factors[i] <- 1 - (rss_f / tss)
}

# Print variance explained by each factor cumulatively
variance_explained_factors
```

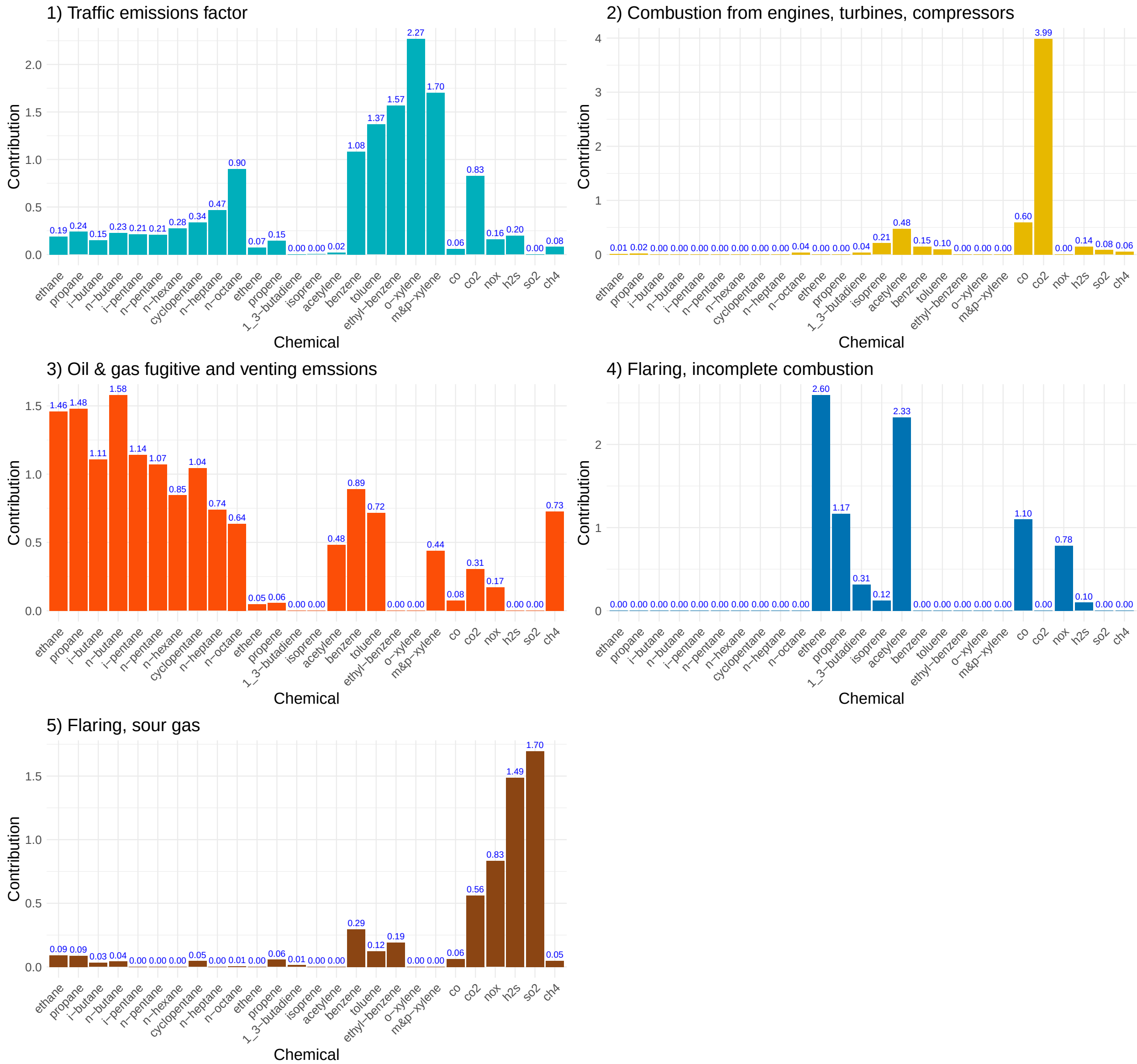
```
## [1] 0.2395401 0.5113683 0.8113445 0.8921360 0.9212864
```

```r
par(mfrow = c(1, 2))
image(basis_matrix_5c_less_o3, main = "Basis Matrix (W)")
image(coef_matrix_5c_less_o3, main = "Coefficient Matrix (H)")
```




```r
# Convert H to a data frame for ggplot
H_df_5c_less_o3 <- as.data.frame(coef_matrix_5c_less_o3)
# Add a column for chemicals
```

```r
H_df_5c_less_o3$Component <- rownames(H_df_5c_less_o3)

# Reshape data to long format
H_long_5c_less_o3 <- pivot_longer(H_df_5c_less_o3, cols = -Component,
                                  names_to = "Chemical", values_to = "Contribution")

# Plot
nmfplt_1_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                            '1', '1) Traffic emissions factor')
nmfplt_2_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                            '2', '2) Combustion from engines, turbines, compressors')
nmfplt_3_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                            '3', '3) Oil & gas fugitive and venting emssions')
nmfplt_4_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                            '4', '4) Flaring, incomplete combustion')
nmfplt_5_svd_5c_less_o3 <- get_component_plot(H_long_5c_less_o3,
                                            '5', '5) Flaring, sour gas')
```



Factor analysis

- merge in factors 1-5 to dataset (hourly)

```
# First look at how well this approximates
fitted_5c_less_o3 <- fitted(nmf_result_5c_less_o3)
sum(abs(normalized_matrix_less_o3-fitted_5c_less_o3))
```

```
## [1] 1059.63
```

```
# NMF factorizes V = WH
# Store Basis matrix (W) and Coef Matrix (H)
saveRDS(basis_matrix_5c_less_o3, 'result_rfiles/nmf_norm_5c_less_o3_basis.rds')
saveRDS(coef_matrix_5c_less_o3, 'result_rfiles/nmf_norm_5c_less_o3_coef.rds')

# Merge basis matrix into hourly observations
basis_matrix_5c_less_o3 <- as_tibble(basis_matrix_5c_less_o3) %>%
  setNames(c('Factor1', 'Factor2', 'Factor3', 'Factor4', 'Factor5'))
```

```
## Warning: The `x` argument of `as_tibble.matrix()` must have unique column names if
## `.name_repair` is omitted as of tibble 2.0.0.
## i Using compatibility `.name_repair`.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.
```

```
normalized_hourly_data_5c_less_o3 <- hourly_nona[,c('day', 'time_utc')] %>%
  cbind(normalized_matrix_less_o3) %>%
  cbind(basis_matrix_5c_less_o3) %>%
  right_join(hourly_data %>% select(-'day'), join_by(time_utc), suffix = c('_norm', ''))

# saveRDS(normalized_hourly_data_5c_less_o3,
#  'result_rfiles/normalized_hourly_data_5c_less_o3.rds')
normalized_hourly_data_5c_less_o3 <- readRDS('result_rfiles/normalized_hourly_data_5c_less_o3.rds')
```

- make daily dataset for VNF analysis
- compute wind directions from plots

```
# Also compute a daily dataset
normalized_daily_data_5c_less_o3 <- normalized_hourly_data_5c_less_o3 %>%
  group_by(day) %>%
  summarise(across(where(is.numeric) & !any_of('wdr_deg'), ~ mean(.x, na.rm = T)),
          wdr_deg = as.numeric(mean(circular(wdr_deg, units = "degrees"), na.rm = T))) %>%
  mutate(wdr_deg = if_else(wdr_deg < 0, wdr_deg+360, wdr_deg)) %>%
  mutate(wind_45_135 = wdr_deg >= 45 & wdr_deg < 135,
         wind_135_180 = wdr_deg >= 135 & wdr_deg < 180,
         wind_180_270 = wdr_deg >= 180 & wdr_deg < 270,
         wind_270_45 = wdr_deg >= 270 & wdr_deg < 45)

# saveRDS(normalized_daily_data_5c_less_o3,
#  'result_rfiles/normalized_daily_data_5c_less_o3.rds')

normalized_daily_data_5c_less_o3 <-
  readRDS('result_rfiles/normalized_daily_data_5c_less_o3.rds')
```

- 1) number of flares in 100km of trailer associated with NMF
- 2) weighted count based on distance to trailer

```
# Check if relationship between # flares and flare factor (4 & 5)
# Linear model
flare_factor <- lm(n_flare_100 ~ Factor1 + Factor2 + Factor3 + Factor4 + Factor5,
                  data = normalized_daily_data_5c_less_o3)
summary(flare_factor)
```

```
##
## Call:
## lm(formula = n_flare_100 ~ Factor1 + Factor2 + Factor3 + Factor4 +
##     Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -54.638 -22.160   4.205  18.488  76.270
##
## Coefficients:
```

```
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   52.438      7.455   7.034 1.61e-11 ***
## Factor1      -27.402    106.172  -0.258   0.7965
## Factor2     -338.560    196.573  -1.722   0.0861 .
## Factor3      286.534    151.310   1.894   0.0593 .
## Factor4     -287.536    244.717  -1.175   0.2410
## Factor5      231.978    212.510   1.092   0.2760
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 27.79 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.03877,    Adjusted R-squared:  0.02117
## F-statistic: 2.202 on 5 and 273 DF,  p-value: 0.05434
```

```
flare_factor45 <- lm(n_flare_100 ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
summary(flare_factor45)
```

```
##
## Call:
## lm(formula = n_flare_100 ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -53.409 -23.830   5.588  18.235  77.131
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   40.780      3.386  12.044   <2e-16 ***
## Factor4      -48.431    150.383  -0.322   0.7477
## Factor5      360.559    206.393   1.747   0.0818 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 28.02 on 276 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.01171,    Adjusted R-squared:  0.004548
## F-statistic: 1.635 on 2 and 276 DF,  p-value: 0.1968
```

```
flare_factor_weighted <- lm(weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 + Factor5,
                            data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 +
##     Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.3295 -0.2180  0.0546  0.3809  3.9848
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   2.2572     0.2278   9.907   <2e-16 ***
```

```
## Factor1       0.1244     3.2450   0.038   0.9694
## Factor2      -4.7740     6.0080  -0.795   0.4275
## Factor3       7.4339     4.6246   1.607   0.1091
## Factor4     -12.9155     7.4794  -1.727   0.0853 .
## Factor5       4.0762     6.4951   0.628   0.5308
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8492 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.02221,    Adjusted R-squared:  0.0043
## F-statistic:  1.24 on 5 and 273 DF,  p-value: 0.2905
```

```
flare_factor_weighted45 <- lm(weighted.count ~ Factor4 + Factor5,
                              data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted45)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2558 -0.1821  0.0775  0.3622  3.9366
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   2.0910     0.1029  20.315   <2e-16 ***
## Factor4      -4.0144     4.5712  -0.878    0.381
## Factor5       7.3663     6.2738   1.174    0.241
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8518 on 276 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.005595,   Adjusted R-squared:  -0.001611
## F-statistic: 0.7765 on 2 and 276 DF,  p-value: 0.461
```

```
# All factors + wind speed + wind direction + factor5:sw wind.
# Wind direction from 270 to 45 is left as reference group.
flare_factor_weighted_2 <- lm(weighted.count ~ Factor1 + Factor2 + Factor3 +
                                Factor4 + Factor5 + wsp_ms + wind_45_135 +
                                wind_135_180 + Factor5*wind_180_270,
                              data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_2)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor1 + Factor2 + Factor3 + Factor4 +
##     Factor5 + wsp_ms + wind_45_135 + wind_135_180 + Factor5 *
##     wind_180_270, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.4382 -0.2036  0.0782  0.3578  3.9528
```

```
##
## Coefficients:
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)                 2.14418    0.33390   6.422 6.11e-10 ***
## Factor1                     0.07365    3.35780   0.022   0.9825
## Factor2                    -4.92773    6.19462  -0.795   0.4270
## Factor3                     8.99603    4.80767   1.871   0.0624 .
## Factor4                   -10.66714    7.82960  -1.362   0.1742
## Factor5                     3.28556    7.52447   0.437   0.6627
## wsp_ms                      0.04430    0.04523   0.980   0.3282
## wind_45_135TRUE            -0.15557    0.17743  -0.877   0.3814
## wind_135_180TRUE           -0.15153    0.13270  -1.142   0.2545
## wind_180_270TRUE           -0.21667    0.22628  -0.958   0.3392
## Factor5:wind_180_270TRUE   2.51821   13.08348   0.192   0.8475
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8524 on 268 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.03302,    Adjusted R-squared:  -0.003061
## F-statistic: 0.9152 on 10 and 268 DF,  p-value: 0.5196
```

```
# Same as above but only factor 4 and 5
flare_factor_weighted_3 <- lm(weighted.count ~ Factor4 + Factor5 + wsp_ms +
                                Factor5*wind_180_270,
                              data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_3)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5 + wsp_ms + Factor5 *
##     wind_180_270, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2706 -0.1961  0.0714  0.3721  3.9358
##
## Coefficients:
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)                2.057728   0.222033   9.268   <2e-16 ***
## Factor4                   -3.273445   5.155494  -0.635    0.526
## Factor5                    7.499668   7.297235   1.028    0.305
## wsp_ms                     0.009441   0.040855   0.231    0.817
## wind_180_270TRUE          -0.059345   0.215638  -0.275    0.783
## Factor5:wind_180_270TRUE -0.078349  12.897092  -0.006    0.995
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.856 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.006554,   Adjusted R-squared:  -0.01164
## F-statistic: 0.3602 on 5 and 273 DF,  p-value: 0.8754
```

```
# Same as above but interaction between factor 4 and SW wind
flare_factor_weighted_3b <- lm(weighted.count ~ Factor4 + Factor5 + wsp_ms +
```

```r
                                 Factor4*wind_180_270,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_3b)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5 + wsp_ms + Factor4 *
##     wind_180_270, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.3058 -0.2123  0.0650  0.3774  3.9523
##
## Coefficients:
##                              Estimate Std. Error t value Pr(>|t|)
## (Intercept)                  2.030311   0.215853   9.406   <2e-16 ***
## Factor4                     -0.841684   5.604781  -0.150    0.881
## Factor5                      7.401203   6.365967   1.163    0.246
## wsp_ms                       0.005478   0.040870   0.134    0.893
## wind_180_270TRUE             0.143565   0.224432   0.640    0.523
## Factor4:wind_180_270TRUE -10.510472   9.618074  -1.093    0.275
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8541 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.01088,    Adjusted R-squared:  -0.007235
## F-statistic: 0.6006 on 5 and 273 DF,  p-value: 0.6995
```

```r
# Same as above but with East wind
flare_factor_weighted_3c <- lm(weighted.count ~ Factor4 + Factor5 + wsp_ms +
                                 Factor5*wind_45_135,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_3c)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5 + wsp_ms + Factor5 *
##     wind_45_135, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2355 -0.1832  0.0761  0.3768  3.9129
##
## Coefficients:
##                             Estimate Std. Error t value Pr(>|t|)
## (Intercept)                2.1177298  0.2207356   9.594   <2e-16 ***
## Factor4                   -4.0986004  5.1120629  -0.802    0.423
## Factor5                    6.1846170  6.5540446   0.944    0.346
## wsp_ms                     0.0008777  0.0407876   0.022    0.983
## wind_45_135TRUE           -0.4275903  0.3752245  -1.140    0.255
## Factor5:wind_45_135TRUE 22.0187173 23.3341439   0.944    0.346
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 0.8543 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.01053,    Adjusted R-squared:  -0.007588
## F-statistic: 0.5813 on 5 and 273 DF,  p-value: 0.7143
```

```r
flare_factor_weighted_3d <- lm(weighted.count ~ Factor4 + Factor5 + wsp_ms +
                                 Factor4*wind_45_135,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_3d)
```

```
##
## Call:
## lm(formula = weighted.count ~ Factor4 + Factor5 + wsp_ms + Factor4 *
##     wind_45_135, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2680 -0.1822  0.0707  0.3665  3.9260
##
## Coefficients:
##                         Estimate Std. Error t value Pr(>|t|)
## (Intercept)              2.09473    0.21997   9.523   <2e-16 ***
## Factor4                 -4.50558    5.36882  -0.839    0.402
## Factor5                  7.78444    6.38818   1.219    0.224
## wsp_ms                   0.00343    0.04074   0.084    0.933
## wind_45_135TRUE         -0.19324    0.28449  -0.679    0.498
## Factor4:wind_45_135TRUE  4.84677   13.38860   0.362    0.718
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8555 on 273 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.007783,   Adjusted R-squared:  -0.01039
## F-statistic: 0.4283 on 5 and 273 DF,  p-value: 0.8288
```

```r
# Wind speed + factor 4 and interaction with East wind
flare_factor_weighted_4a <- lm(weighted.count ~ wsp_ms + Factor4*wind_45_135,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_4a)
```

```
##
## Call:
## lm(formula = weighted.count ~ wsp_ms + Factor4 * wind_45_135,
##     data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.1668 -0.1983  0.0661  0.3882  3.8663
##
## Coefficients:
##                          Estimate Std. Error t value Pr(>|t|)
## (Intercept)              2.187226   0.206642  10.585   <2e-16 ***
## wsp_ms                  -0.003785   0.040343  -0.094    0.925
## Factor4                 -2.428778   5.095632  -0.477    0.634
## wind_45_135TRUE         -0.171010   0.284161  -0.602    0.548
```

```
## Factor4:wind_45_135TRUE  3.879541  13.376874   0.290    0.772
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8562 on 274 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.002386,   Adjusted R-squared:  -0.01218
## F-statistic: 0.1638 on 4 and 274 DF,  p-value: 0.9565
```

```
# Wind speed + factor 4 and interaction with SE wind
flare_factor_weighted_4b <- lm(weighted.count ~ wsp_ms + Factor4*wind_135_180,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_4b)
```

```
##
## Call:
## lm(formula = weighted.count ~ wsp_ms + Factor4 * wind_135_180,
##     data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2269 -0.2186  0.0794  0.3693  3.8404
##
## Coefficients:
##                           Estimate Std. Error t value Pr(>|t|)
## (Intercept)               2.229232   0.202818  10.991   <2e-16 ***
## wsp_ms                    0.001297   0.039954   0.032   0.9741
## Factor4                  -5.716640   5.512131  -1.037   0.3006
## wind_135_180TRUE         -0.440258   0.229503  -1.918   0.0561 .
## Factor4:wind_135_180TRUE 18.354002   9.757795   1.881   0.0610 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.851 on 274 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.01456,   Adjusted R-squared:  0.0001782
## F-statistic: 1.012 on 4 and 274 DF,  p-value: 0.4014
```

```
# Wind speed + factor 4 and interaction with SW wind
flare_factor_weighted_4c <- lm(weighted.count ~ wsp_ms + Factor4*wind_180_270,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_4c)
```

```
##
## Call:
## lm(formula = weighted.count ~ wsp_ms + Factor4 * wind_180_270,
##     data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.1911 -0.1952  0.0539  0.4087  3.8937
##
## Coefficients:
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)                2.121372   0.201270  10.540   <2e-16 ***
## wsp_ms                    -0.001567   0.040444  -0.039    0.969
```

```
## Factor4                      1.058349   5.364665   0.197    0.844
## wind_180_270TRUE             0.143445   0.224576   0.639    0.524
## Factor4:wind_180_270TRUE -10.634150   9.623656  -1.105    0.270
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8547 on 274 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.005983,   Adjusted R-squared:  -0.008528
## F-statistic: 0.4123 on 4 and 274 DF,  p-value: 0.7997
```

```
# Wind speed + factor 5 and interaction with East wind
flare_factor_weighted_5a <- lm(weighted.count ~ wsp_ms + Factor5*wind_45_135,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_5a)
```

```
##
## Call:
## lm(formula = weighted.count ~ wsp_ms + Factor5 * wind_45_135,
##     data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2299 -0.1901  0.0789  0.3725  3.9421
##
## Coefficients:
##                          Estimate Std. Error t value Pr(>|t|)
## (Intercept)               2.01637    0.18083  11.151   <2e-16 ***
## wsp_ms                    0.01530    0.03658   0.418    0.676
## Factor5                   4.62551    6.25483   0.740    0.460
## wind_45_135TRUE          -0.40644    0.37405  -1.087    0.278
## Factor5:wind_45_135TRUE 21.30900   23.30214   0.914    0.361
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8537 on 274 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.008204,   Adjusted R-squared:  -0.006275
## F-statistic: 0.5666 on 4 and 274 DF,  p-value: 0.6871
```

```
# Wind speed + factor 5 and interaction with SE wind
flare_factor_weighted_5b <- lm(weighted.count ~ wsp_ms + Factor5*wind_135_180,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_5b)
```

```
##
## Call:
## lm(formula = weighted.count ~ wsp_ms + Factor5 * wind_135_180,
##     data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2259 -0.1876  0.0693  0.3775  3.9290
##
## Coefficients:
##                           Estimate Std. Error t value Pr(>|t|)
```

```
## (Intercept)               2.02295    0.18889  10.710   <2e-16 ***
## wsp_ms                    0.01822    0.03643   0.500    0.618
## Factor5                   4.19811    7.25463   0.579    0.563
## wind_135_180TRUE         -0.15866    0.20317  -0.781    0.436
## Factor5:wind_135_180TRUE  6.06208   12.22399   0.496    0.620
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8545 on 274 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.006345,   Adjusted R-squared:  -0.008161
## F-statistic: 0.4374 on 4 and 274 DF,  p-value: 0.7816
```

```r
# Wind speed + factor 5 and interaction with SW wind
flare_factor_weighted_5c <- lm(weighted.count ~ wsp_ms + Factor5*wind_180_270,
                               data = normalized_daily_data_5c_less_o3)
summary(flare_factor_weighted_5c)
```

```
##
## Call:
## lm(formula = weighted.count ~ wsp_ms + Factor5 * wind_180_270,
##     data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2696 -0.2009  0.0671  0.3748  3.9556
##
## Coefficients:
##                          Estimate Std. Error t value Pr(>|t|)
## (Intercept)               1.98021    0.18525  10.689   <2e-16 ***
## wsp_ms                    0.02098    0.03655   0.574    0.566
## Factor5                   6.25646    7.02199   0.891    0.374
## wind_180_270TRUE         -0.06960    0.21480  -0.324    0.746
## Factor5:wind_180_270TRUE -0.16687   12.88229  -0.013    0.990
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8551 on 274 degrees of freedom
##   (1 observation deleted due to missingness)
## Multiple R-squared:  0.005087,   Adjusted R-squared:  -0.009438
## F-statistic: 0.3502 on 4 and 274 DF,  p-value: 0.8438
```

```r
# Check relationship between avg flare distance and flare factor (4 & 5)
# Linear model
flare_factor_dist <- lm(distToLovi ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
summary(flare_factor_dist)
```

```
##
## Call:
## lm(formula = distToLovi ~ Factor4 + Factor5, data = normalized_daily_data_5c_less_o3)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -34.449  -2.443  -0.139   2.266  31.399
##
```

```
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  54.7821     0.8756  62.564   <2e-16 ***
## Factor4       7.2656    39.7289   0.183    0.855
## Factor5      64.5797    52.2590   1.236    0.218
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.883 on 252 degrees of freedom
##   (25 observations deleted due to missingness)
## Multiple R-squared:  0.008425,   Adjusted R-squared:  0.0005557
## F-statistic: 1.071 on 2 and 252 DF,  p-value: 0.3444
```