Repeat evaluation of ALFAM2 parameter set 1

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Overview

This document for Arman Favrot presents a repeat of the evaluation of the ALFAM2 model with parameter set 1 originally presented in the 2019 paper introducing the model.

Packages and functions

```
library(data.table)
library(ALFAM2)
source('dfsumm.R')
source('model_stats.R')
```

See ALFAM2 version.

```
packageVersion('ALFAM2')
```

```
## [1] '3.58'
```

The problem you found with duplicated columns should not be present in this version, which is available from the dev branch now. But note that the function does not add dummy variable columns for "reference levels", and both cattle manure and trailing hose are reference levels, so that behavior was not an error.

Input data

Get pmid from paper.

```
pmidcal <- fread('../data/S1_plot_codes_calibration.csv')
pmideval <- fread('../data/S2_plot_codes_evaluation.csv')</pre>
```

To associate these with measurements below, combine them in a data table here.

```
pmidcal[, datasub := 'cal']
pmideval[, datasub := 'eval']
pmid <- rbind(pmidcal, pmideval)</pre>
```

Load interval-level data. Note this is version 1.0 of ALFAM2 "database". See https://github.com/sashahafn er/ALFAM2-data/tree/cfa0055e44907578bf40e0eac389e020f93dd6b1/data%20-%20ALFAM2%20output for this version. Unfortunately I was just getting started with GitHub releases around this time in 2018, so there is no release for this version. Since then the situation has improved. Now you can always find the database version in data-output/... (here), and new versions get releases (here).

```
idat <- fread('../data/ALFAM2_interval.csv')</pre>
```

Fix changed variable name.

```
idat[, app.mthd := app.method]
Merge in pmid and subset keys.
dim(idat)
## [1] 30907
               110
idat <- merge(idat, pmid, by = 'pmid')</pre>
dim(idat)
## [1] 12193
               111
Trim to 78 hours.
idat <- idat[ct > 0 & ct < 78, ]
Check values.
dfsumm(idat[datasub == 'eval',.(pmid, app.mthd, app.rate, man.dm, man.source, air.temp, wind.2m,
                                 man.ph, rain.rate, incorp)])
##
## 423 rows and 10 columns
## 413 unique rows
##
                          pmid app.mthd app.rate man.dm man.source air.temp
## Class
                       integer character numeric numeric character numeric
## Minimum
                           195
                                      bc
                                              6.6
                                                      1.52
                                                                            0.3
                                                                  cat
## Maximum
                          1900
                                      ts
                                              58.2
                                                      10.7
                                                                  pig
                                                                           34.1
                                                                           15.1
## Mean
                          1300
                                    <NA>
                                              29.3
                                                      6.07
                                                                  <NA>
## Unique (excld. NA)
                            48
                                                45
                                                        45
                                                                     2
                                                                            207
                                                 0
## Missing values
                             0
                                       0
                                                         0
                                                                     Λ
                                                                              1
## Sorted
                          TRUE
                                   FALSE
                                            FALSE
                                                     FALSE
                                                                FALSE
                                                                          FALSE
##
                       wind.2m man.ph rain.rate
                                                     incorp
## Class
                       numeric numeric
                                         numeric character
## Minimum
                          0.22
                                   6.8
                                                0
                                                       none
## Maximum
                          16.8
                                   8.2
                                             3.08
                                                       none
                          3.08
                                  7.38
                                           0.0744
## Mean
                                                       <NA>
## Unique (excld. NA)
                           267
                                    22
                                               44
                                                          1
## Missing values
                             2
                                    39
                                              134
                                                          0
                                                       TRUE
## Sorted
                         FALSE
                                 FALSE
                                           FALSE
##
dfsumm(idat[datasub == 'cal',.(pmid, app.mthd, app.rate, man.dm, man.source, air.temp, wind.2m,
                                man.ph, rain.rate, incorp)])
##
    5501 rows and 10 columns
##
##
   5386 unique rows
                          pmid app.mthd app.rate man.dm man.source air.temp
## Class
                       integer character numeric numeric character numeric
## Minimum
                           182
                                      bc
                                               7.9
                                                         1
                                                                           -1.9
                                                                  cat
## Maximum
                          1900
                                      ts
                                               133
                                                      13.6
                                                                  pig
                                                                           35.2
## Mean
                          1350
                                    <NA>
                                              48.2
                                                      5.93
                                                                  <NA>
                                                                           13.1
## Unique (excld. NA)
                           490
                                       4
                                               202
                                                       208
                                                                     2
                                                                            958
## Missing values
                                       0
                                                                     0
                                                                              3
                             0
                                                 0
                                                         0
## Sorted
                          TRUE
                                   FALSE
                                            FALSE
                                                     FALSE
                                                                FALSE
                                                                          FALSE
```

```
##
##
                      wind.2m man.ph rain.rate
                                                     incorp
## Class
                      numeric numeric
                                         numeric character
## Minimum
                       0.0513
                                   6.4
                                               0
                                                       deep
## Maximum
                          16.8
                                   8.5
                                             7.1
                                                    shallow
## Mean
                          3.09
                                  7.32
                                          0.0511
                                                       <NA>
## Unique (excld. NA)
                          1782
                                    65
                                              314
## Missing values
                            13
                                  1053
                                            1204
                                                          0
## Sorted
                         FALSE
                                 FALSE
                                           FALSE
                                                      FALSE
##
```

Fill in missing wind speed, air temperature, rainfall values. This is a thorny problem. Dropping values means leaving out emission intervals. Here they are set to the average by plot, or, for rain, zero.

```
idat[, wind.2m.ave := mean(wind.2m, na.omit = TRUE), by = pmid]
idat[, air.temp.ave := mean(air.temp, na.omit = TRUE), by = pmid]

idat[is.na(wind.2m), wind.2m := wind.2m.ave]
idat[is.na(air.temp), air.temp := air.temp.ave]

idat[is.na(rain.rate), rain.rate := 0]
idat[is.na(rain.cum), rain.cum := 0]
```

Check values.

```
##
   423 rows and 10 columns
##
   413 unique rows
##
                          pmid app.mthd app.rate man.dm man.source air.temp
## Class
                       integer character numeric numeric character numeric
## Minimum
                          195
                                      bc
                                              6.6
                                                      1.52
                                                                  cat
                                                                            0.3
## Maximum
                          1900
                                              58.2
                                                      10.7
                                                                           34.1
                                      ts
                                                                  pig
                          1300
                                              29.3
                                                      6.07
                                                                 <NA>
## Mean
                                    <NA>
                                                                           15.1
## Unique (excld. NA)
                                                45
                                                                     2
                                                                            208
                            48
                                       4
                                                        45
## Missing values
                             0
                                       0
                                                0
                                                         0
                                                                     0
                                                                              0
## Sorted
                          TRUE
                                   FALSE
                                            FALSE
                                                     FALSE
                                                                FALSE
                                                                          FALSE
##
##
                      wind.2m man.ph rain.rate
                                                     incorp
## Class
                      numeric numeric
                                         numeric character
## Minimum
                         0.22
                                   6.8
                                                0
                                                       none
## Maximum
                          16.8
                                   8.2
                                            3.08
                                                       none
## Mean
                          3.09
                                  7.38
                                          0.0508
                                                       <NA>
## Unique (excld. NA)
                           269
                                    22
                                               44
                                                          1
## Missing values
                             0
                                    39
                                                          0
                                                0
## Sorted
                         FALSE
                                 FALSE
                                           FALSE
                                                       TRUE
```

```
##
## 5501 rows and 10 columns
## 5386 unique rows
## pmid app.mthd app.rate man.dm man.source air.temp
```

##	Class	integer	character	numeric	numeric	character	numeric
##	Minimum	182	bc	7.9	1	cat	-1.9
##	Maximum	1900	ts	133	13.6	pig	35.2
##	Mean	1350	<na></na>	48.2	5.93	<na></na>	13.1
##	Unique (excld. NA)	490	4	202	208	2	960
##	Missing values	0	0	0	0	0	0
##	Sorted	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE
##							
##		wind.2m	man.ph ra	ain.rate	incorp		
##	Class	numeric	numeric	numeric	character		
##	Minimum	0.0513	6.4	0	deep		
##	Maximum	16.8	8.5	7.1	shallow		
##	Mean	3.09	7.32	0.0399	<na></na>		
##	Unique (excld. NA)	1794	65	314	3		
##	Missing values	0	1053	0	0		
##	Sorted	FALSE	FALSE	FALSE	FALSE		
##							

Model application

Get parameters without pH. The pH parameters only apply to acidified slurry in set 1. This has changed in set 2 and the new set 3.

```
pars <- alfam2pars01[!grepl('man.ph', names(alfam2pars01))]</pre>
##
               int.f0
                                  int.r1
                                                      int.r2
                                                                         int.r3
          -0.7364889
##
                              -1.1785848
                                                 -0.9543731
                                                                     -2.9012937
##
      app.mthd.os.f0
                                                  man.dm.f0
                             app.rate.f0
                                                                incorp.deep.f4
##
          -1.1717859
                              -0.0134681
                                                  0.4074660
                                                                     -3.6477259
##
   incorp.shallow.f4
                          app.mthd.bc.r1
                                                  man.dm.r1
                                                                    air.temp.r1
##
          -0.4121023
                               0.6283396
                                                 -0.0758220
                                                                      0.0492777
##
          wind.2m.r1
                             air.temp.r3
                                             incorp.deep.r3
                                                                app.mthd.os.r3
##
           0.0486651
                               0.0152419
                                                 -0.3838862
                                                                     -0.1228830
##
        rain.rate.r2
                             rain.cum.r3
           0.4327281
                              -0.0300936
```

Generate predictions. Note group argument allows application to multiple plots. See the vignette for more details. So you can apply the function to any number of plots/locations with a single call. And in this version of the package prep.dum = TRUE by default (new argument name too).

```
pred <- alfam2(idat, pars = pars, app.name = 'tan.app', time.incorp = 'time.incorp', group = 'pmid')</pre>
```

User-supplied parameters are being used.

Incorporation applied for groups: 1500, 1501, 1506, 1515, 1516, 1517, 1518, 1754, 1757, 1760, 1761, head(pred)

```
##
     pmid app.mthd.ts app.mthd.bc app.mthd.os app.mthd.cs incorp.shallow
## 1
     182
                     0
## 2
      182
                     0
                                                0
                                                             0
                                                                             1
                                   1
                     0
## 3
      182
                                   1
                                                0
                                                             0
                                                                             1
                     0
                                                0
                                                             0
## 4
      183
                                   1
                                                                             1
## 5
      183
                     0
                                   1
                                                0
                                                             0
                                                                             1
## 6 183
                                   1
                                                                             1
```

```
##
    incorp.deep man.source.pig
                              ct
                                     dt
## 1
                           0 4.00 4.00 2.267818e+00 104.28139 15.560788
             0
## 2
             0
                           0 21.00 17.00 1.500120e-02 103.48296 18.612039
             0
## 3
                           0 44.75 23.75 3.504149e-07 101.03236 21.077637
## 4
             0
                           0 6.00 6.00 1.722933e+00 52.38892
                                                             4.208149
             Λ
## 5
                           0 20.50 14.50 9.638577e-02 52.43933
                                                             5.784289
## 6
                           0 45.20 24.70 5.636323e-04 51.01390
##
        e.int
                                        f0
                                                 r1
                                                          r2
                                                                      r3
                     j
## 1 15.560788 3.89019706 0.12743255 0.1731848 0.44709929 0.1110777 0.0010605843
    3.051251 0.17948535 0.15242027 0.1731848 0.18412484 0.1110777 0.0009297968
## 3 2.465597 0.10381463 0.17261188 0.1731848 0.33701888 0.1120136 0.0010106235
    4.208149 0.70135819 0.07215619 0.1427583 0.15147475 0.1110777 0.0012895630
    1.576139 0.10869927 0.09918190 0.1427583 0.08777916 0.1110777 0.0011249975
##
    f4 r5
## 1
     1 0
## 2
    1
       Ω
## 3
    1 0
## 4 1 0
## 5 1
## 6 1 0
```

See the dummy variables in the output.

Add predictions to the input variable data frame.

```
idat[, `:=` (j.NH3.pred = pred$j, e.cum.pred = pred$e, e.rel.pred = pred$er)]
```

And get final values (not beyond 78 hours).

```
idat[, ct.max := max(ct), by = pmid]
idat.final <- idat[ct == ct.max, ]</pre>
```

Model fit

Flux.

```
## datasub n me mae mbe
## 1: cal 5501 0.6865335 0.4530807 -0.19009152
## 2: eval 423 0.6641409 0.4279645 -0.09822768
```

Cumulative emission.

datasub n me.cum me.rel mae.cum mae.rel mbe.cum mbe.rel

1: cal 490 0.6095949 0.5284758 6.64300 0.1179259 -2.983639 -0.05565297
2: eval 48 0.6184073 0.5806177 5.64609 0.1138731 -2.808678 -0.04425160

 summ