

Criteria-based approach for optimization of PMF solutions

A case study: ACSM data from Zurich

Criteria-based selection tool in SoFi-6

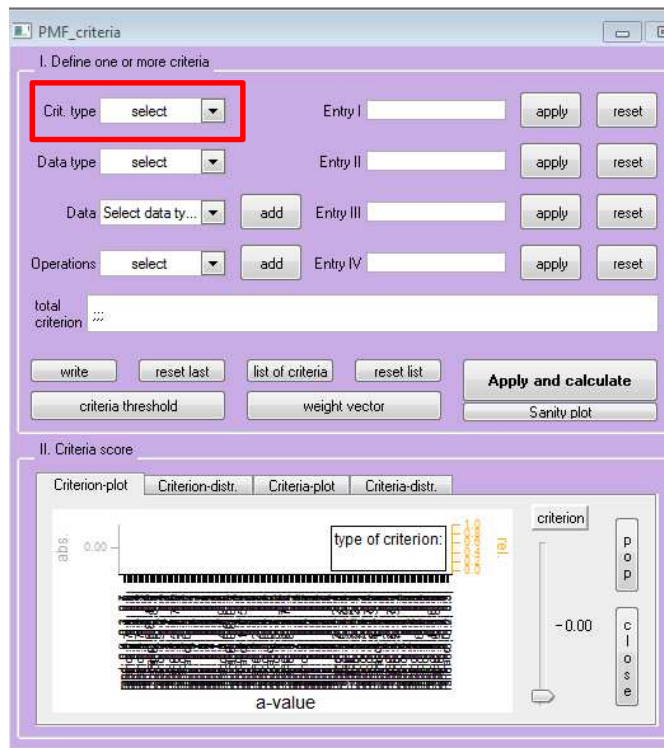
- Criteria-based selection (optimization) tool is a part of the SoFi-6 software package.
- It is not included into the standard (free) package (a manual choice only).
- Can be provided upon request by PSI
- Ask Francesco Canonaco or Andre Prevot

Criteria-based selection tool in SoFi-6

The image displays three windows from the SoFi-6 software interface:

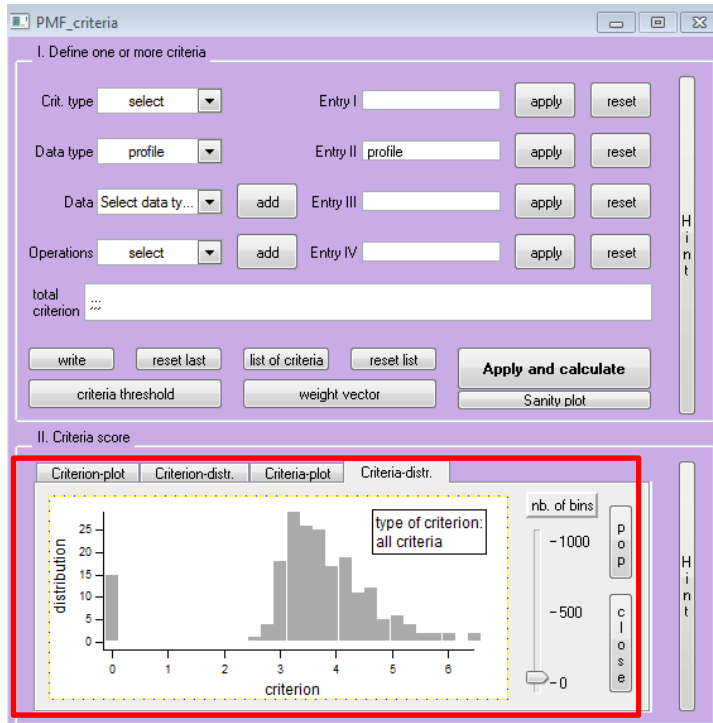
- SoFi_panel:** The main control window. It has tabs for 'Import data', 'Pre-treatment', 'PMF run', and 'PMF result'. Under 'PMF run', there are three steps: 1) Define path of ME2.exe file (Path: C:\ME2_engine5\), 2) Select HDF5 files (II.a Select HDF5 file(s) and II.b Import the chosen HDF5 file(s) into Igor), and 3) Select and analyze PMF solution(s) (III.a Select PMF solution(s) from HDF5 file(s)). A red box highlights step III.a, with a red arrow pointing to the 'PMF solution(s)' button.
- Select_PMFruns:** The 'Settings' window. It has a 'Choice based on:' dropdown set to 'criteria-based', a 'Select HDF5 file:' dropdown set to 'zurich_spring', and an 'x-axis type:' dropdown set to 'a-value'. A red box highlights these three dropdowns, with a red arrow pointing to the 'Criteria-based approach' button.
- PMF_criteria:** The 'Criteria' configuration window. It is divided into two sections: 'I. Define one or more criteria' and 'II. Criteria score'. Section I includes dropdowns for 'Crit. type', 'Data type', and 'Operations', along with four 'Entry' fields (I-IV) and 'apply'/'reset' buttons. Section II includes a 'Criterion-plot' tab showing a bar chart of 'abs.' values for 'a-value' and a 'type of criterion:' dropdown set to 'fcl'. A 'Sanity plot' button is also visible.

Types of criteria and expression



- Maximum / minimum
- R- or R²-Pearson
- Linear Regression
- Can be defined for
 - one factor or a linear combination
 - time series or diurnal cycles
 - hours
 - profile
 - variable or explained variation

Criteria-based selection



- Criteria relative weights
- To position unconstrained factors
- Hard criteria (threshold values)
- Soft criteria (cut-off of the solutions with maximum scores)
- Manual choice (a marquee selection from different histograms)

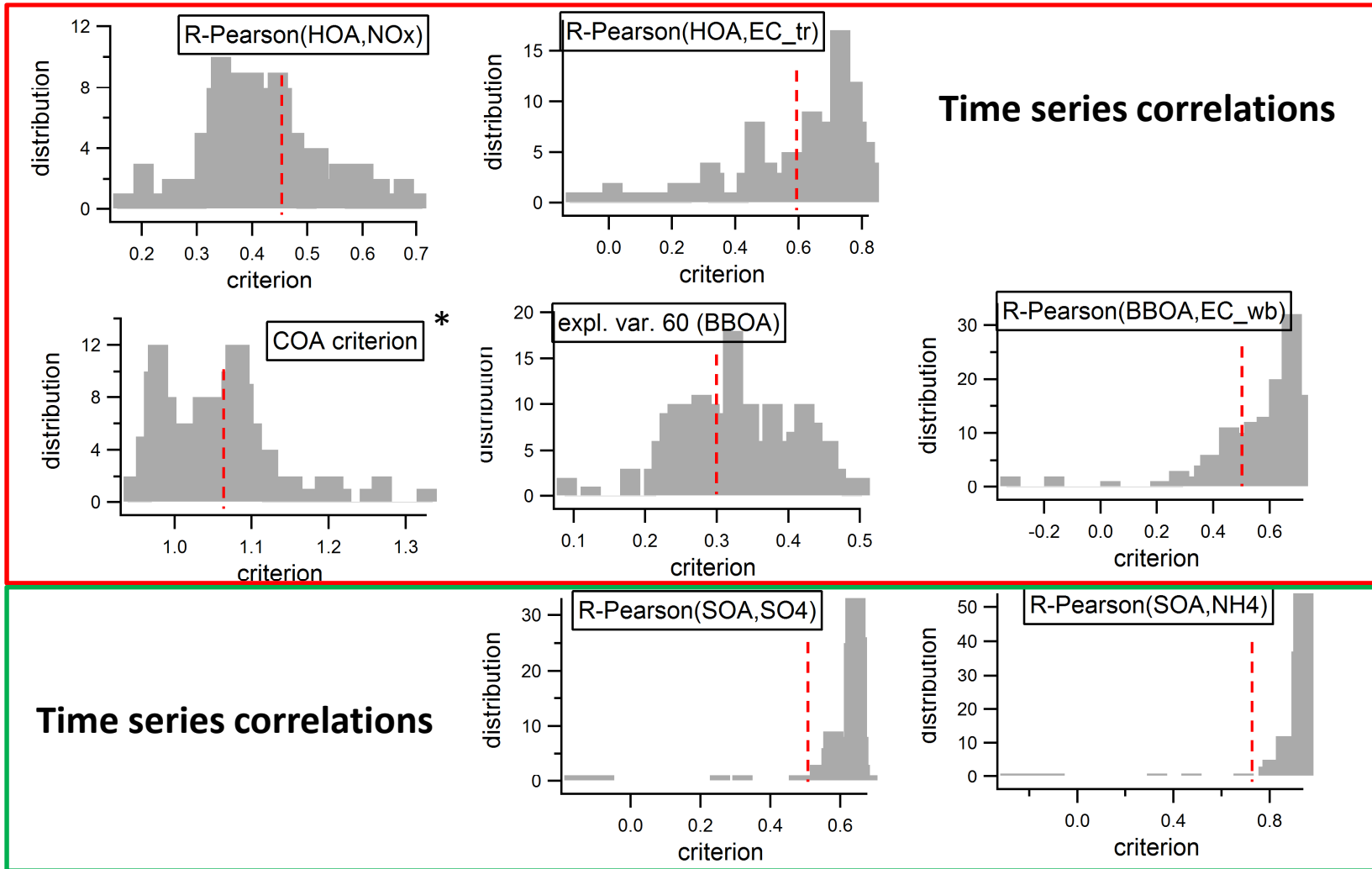
A case study: ACSM data from Zurich

- ACSM data from measurements at Kaserne, a Nabel station in Zurich, in 2011 - 2012
- 4 factors (HOA, COA, BBOA, OOA) in winter season
- 5 factors (HOA, COA, BBOA, two OOA) in spring
- 100 constrained PMF runs for 4- and 5-factor models
- 100 x 2 random combinations of constraining parameters (a-values for HOA, COA and BBOA)
- Results of the 200 runs in one HDF5-file

1: criteria definition and calculation

Criteria distributions and thresholds

winter data

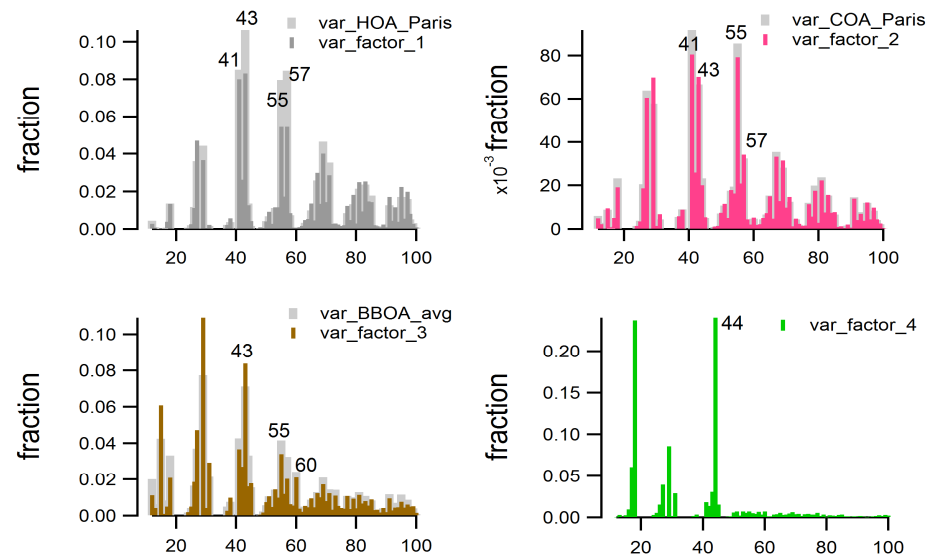


$$*COA\ criterion = \frac{hr[11] + hr[12] + hr[13]}{hr[9] + hr[10] + hr[14] + hr[15]} \times \frac{4}{3}$$

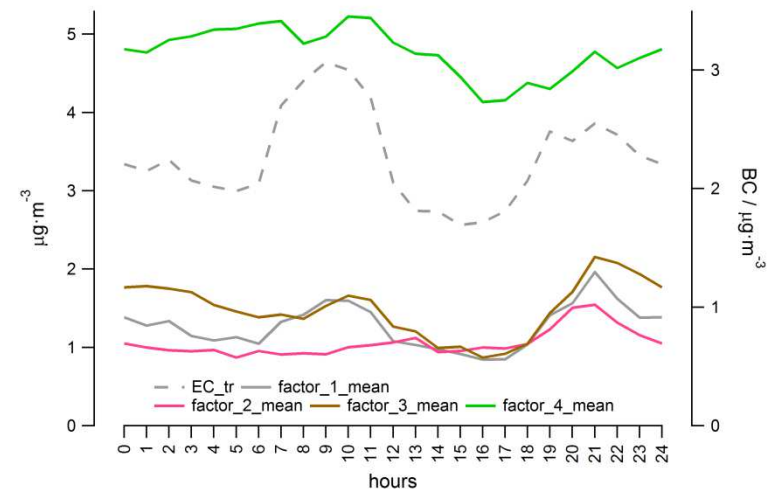
2: criteria-based selected solutions

Factor profiles and diurnal cycles of the “best” solutions

winter data



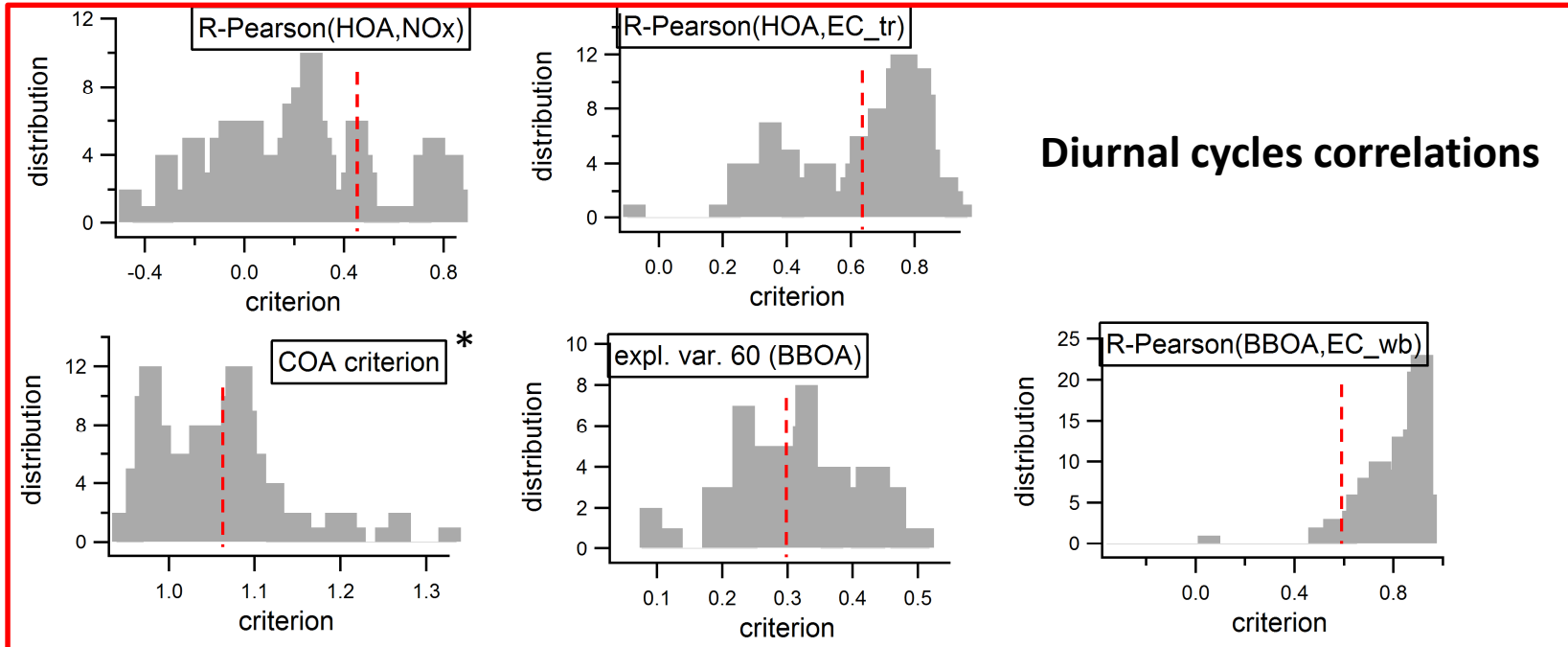
9 solutions based on time series correlation



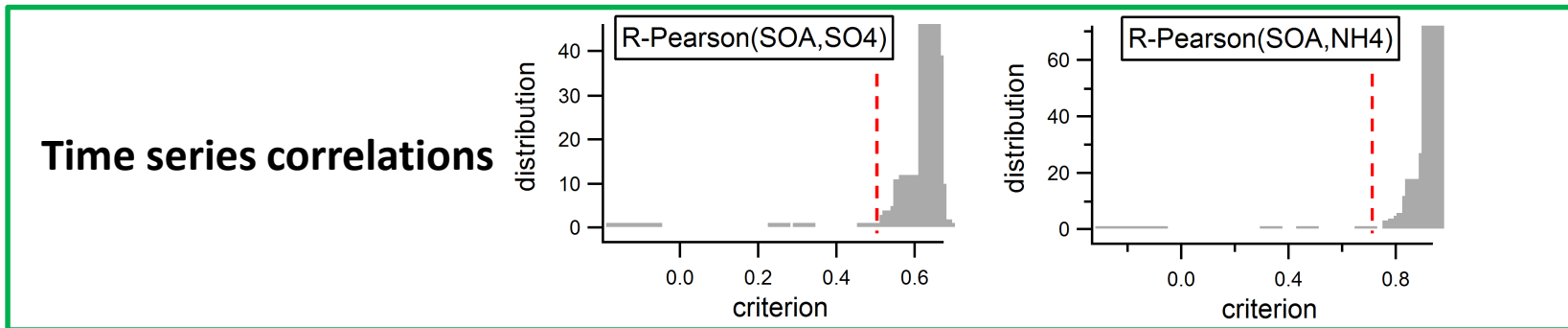
1: criteria definition and calculation

Criteria distributions and thresholds

winter data



Primary factors



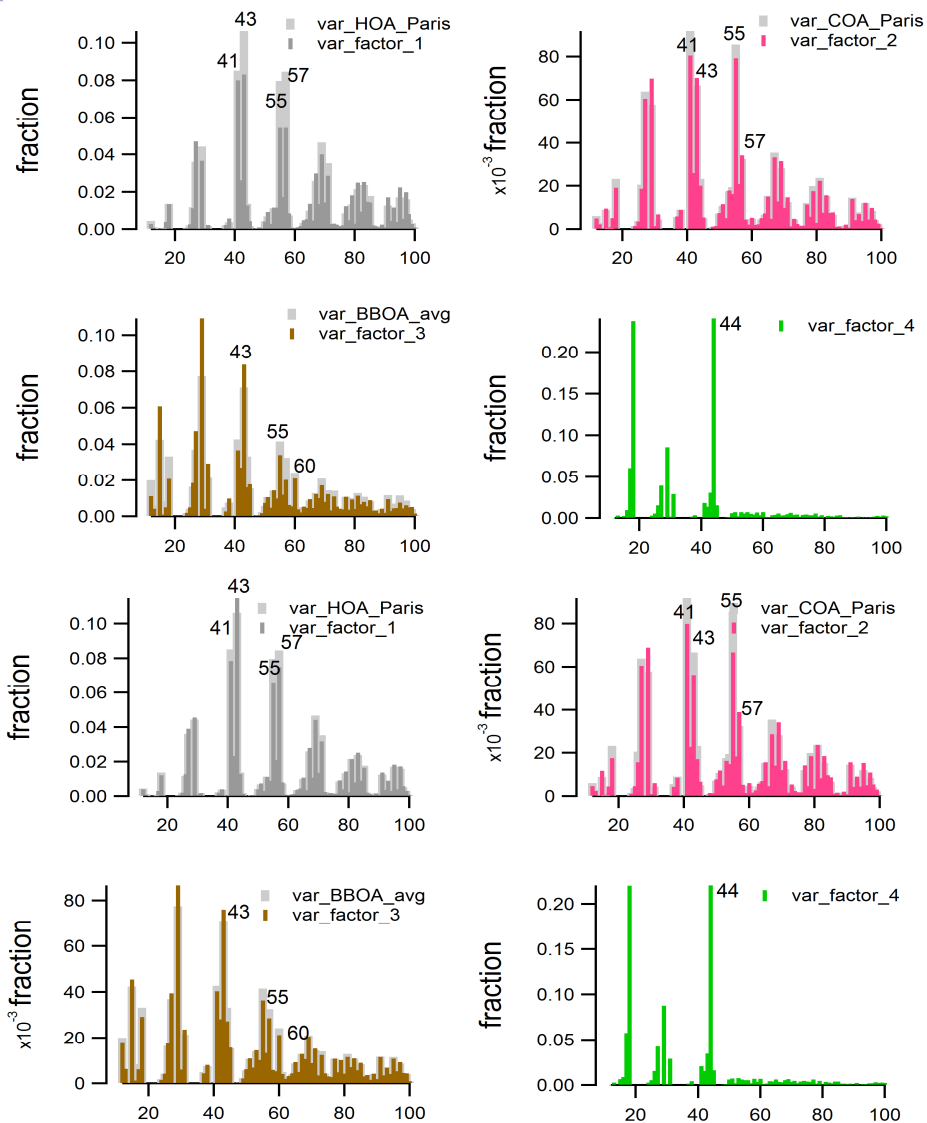
Secondary factors

$$*COA\ criterion = \frac{hr[11] + hr[12] + hr[13]}{hr[9] + hr[10] + hr[14] + hr[15]} \times \frac{4}{3}$$

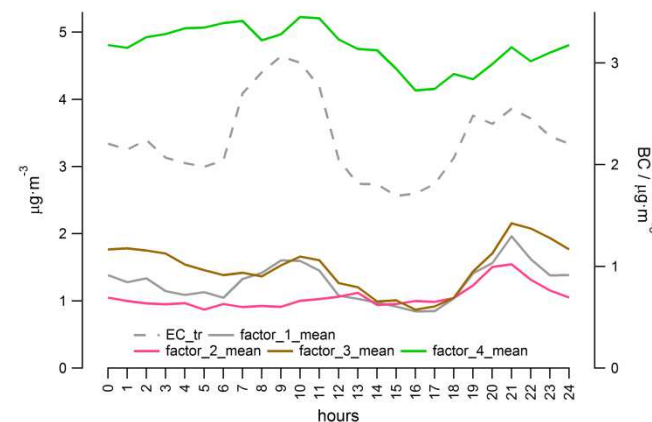
2: criteria-based selected solutions

Factor profiles and diurnal cycles of the “best” solutions

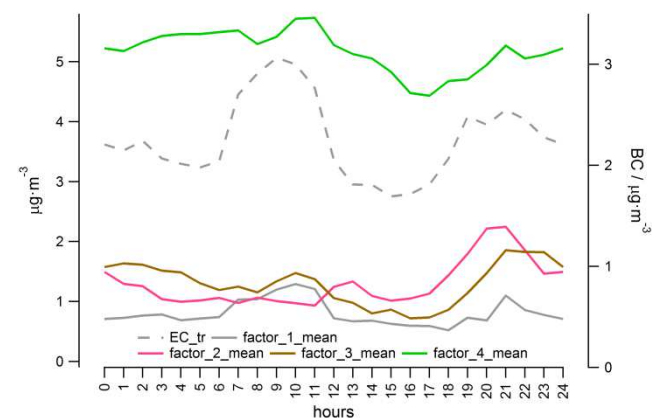
winter data



9 solutions based on time series correlation



3 solutions based on diurnal correlation

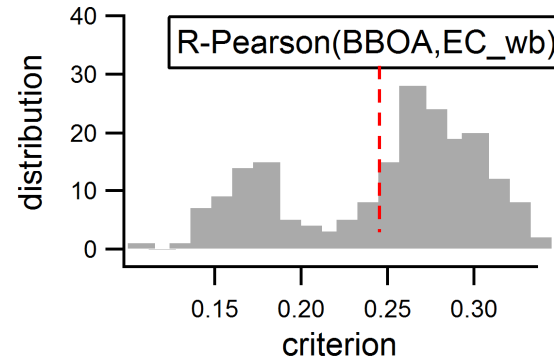
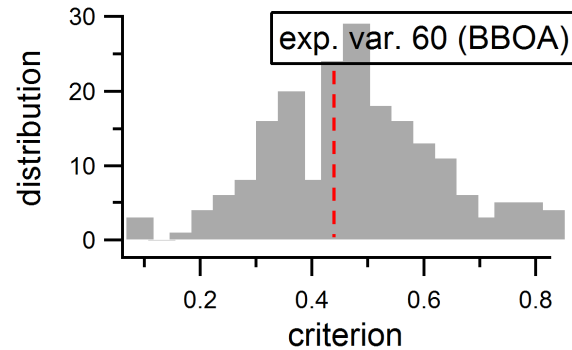
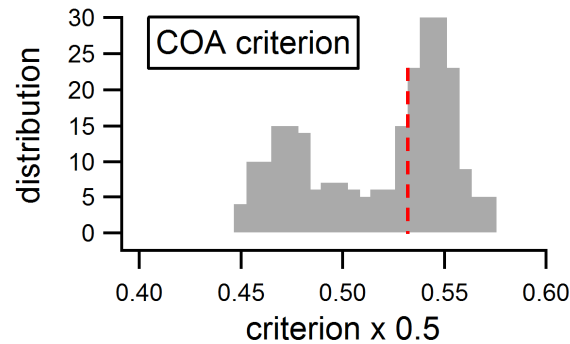
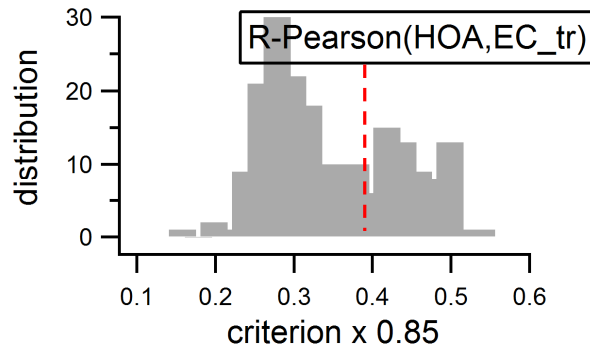


1: criteria definition and calculation

Criteria distributions and thresholds

spring data

Primary factors



$$\text{COA criterion} = \frac{hr[11] + hr[12] + hr[13]}{hr[9] + hr[10] + hr[14] + hr[15]} \times \frac{4}{3}$$

Secondary factors

SV-OOA criteria =

$$\max_{SOA} \left[\frac{f_{43}}{f_{44}} \right]$$

$$\min_{SOA} \left[\frac{f_{44}}{f_{43}} \right]$$

$R(SOA, NO3)$

LV-OOA criteria =

$$\max_{SOA} \left[\frac{f_{44}}{f_{43}} \right]$$

$$\min_{SOA} \left[\frac{f_{43}}{f_{44}} \right]$$

$R(SOA, SO4)$

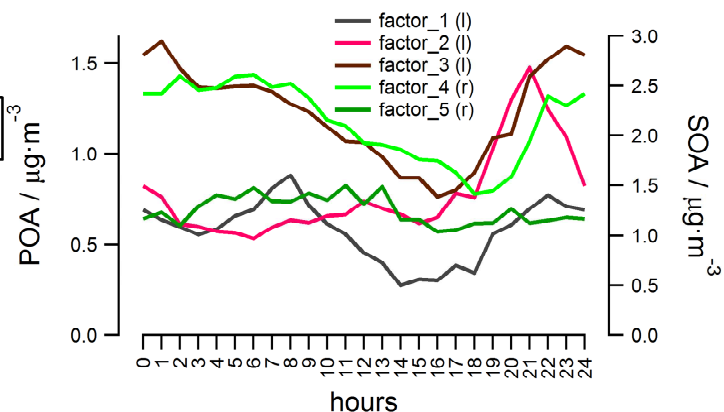
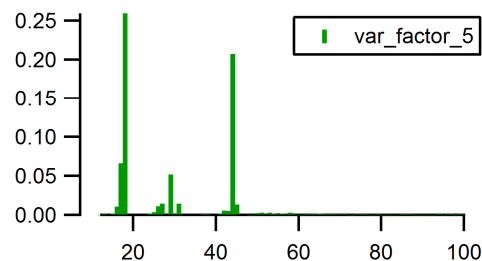
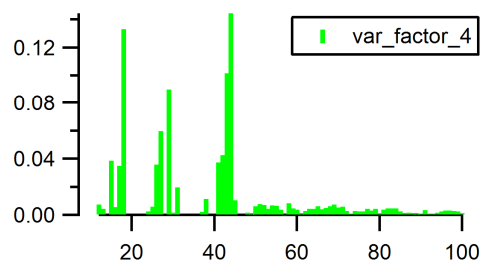
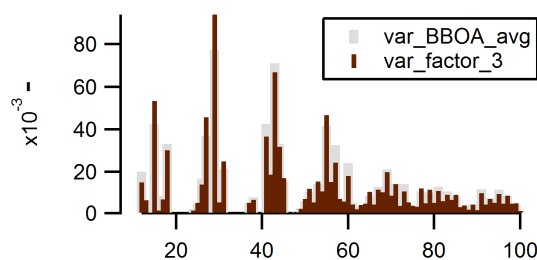
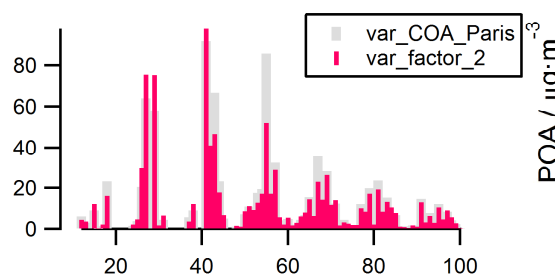
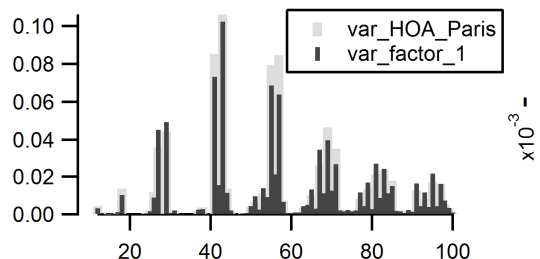
OOA criterion =

$R(OOA, NH4)$

2: criteria-based selected solutions

Factor profiles and diurnal cycles of the “best” solutions

spring data



# sol.	a-value HOA	a-value COA	a-value BBOA
1	0.1	0.3	0.6
2	0.7	0.6	0.1
3	0.5	0.4	0.3
4	0.3	0.3	0.5
5	0.3	0.4	0.3
6	0.6	0.9	0.1
7	0.5	0.3	0.3
8	0.5	0.6	0.4
9	0.6	0.5	0.2
avg.	0.5±0.2	0.5±0.2	0.3±0.2

Conclusion / outlook

- Hard and soft criteria can be combined to select PMF solutions that best represent the data.
- Ca. 10% or less belong to the group of the “best” solutions.
- A seasonal dependence of the criteria distribution needs to be investigated.