ML4AQ meeting – First results with KFAN and ML

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What has been done?

- Modification of the MOS scripts to work in CAMS50-like operational conditions (i.e. daily 4-days forecasts)
- Test of several MOS approaches :
  - MA<N> : moving average on N previous days
  - KF<s/d> : optimcal <static/dynamic> Kalman filter
  - AN<X> : analogs with configuration X
  - KFAN<X> : analogs with configuration X in Kalman space
  - ML<X> : machine learning with algorithm X
- Entire IP domain (only stations with >75% data retained)
- Many changes of my MOS script (e.g. operational-like mode, various MN4 issues to handle, additional flexibility for parallelisation)
- Experiments :
  - MONARCH b007 (2015, without the 2 bugged months)
  - NB : Problem with CAMS50 : no meteorological variables!
- Most of my R scripts are translated to python (results shown today are with the R version)

MONARCH alone (IP domain)

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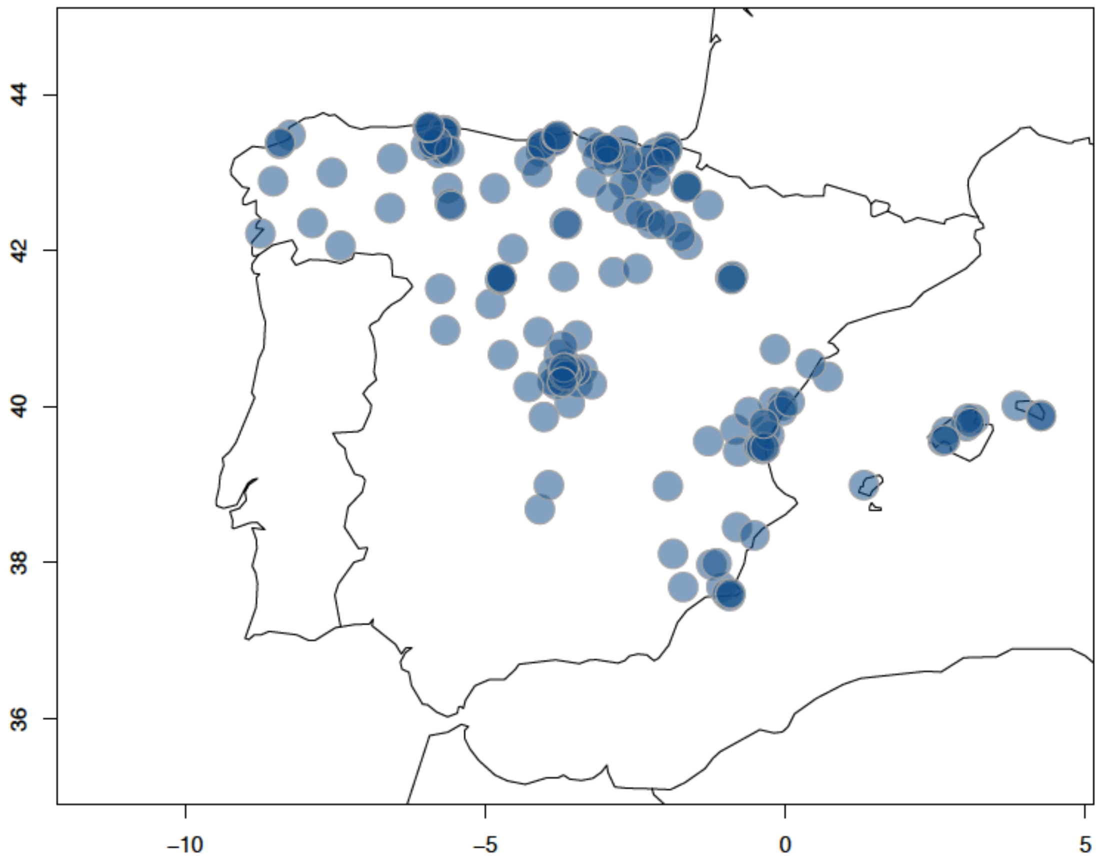
Statistical performance of MONARCH (PM10/IP)



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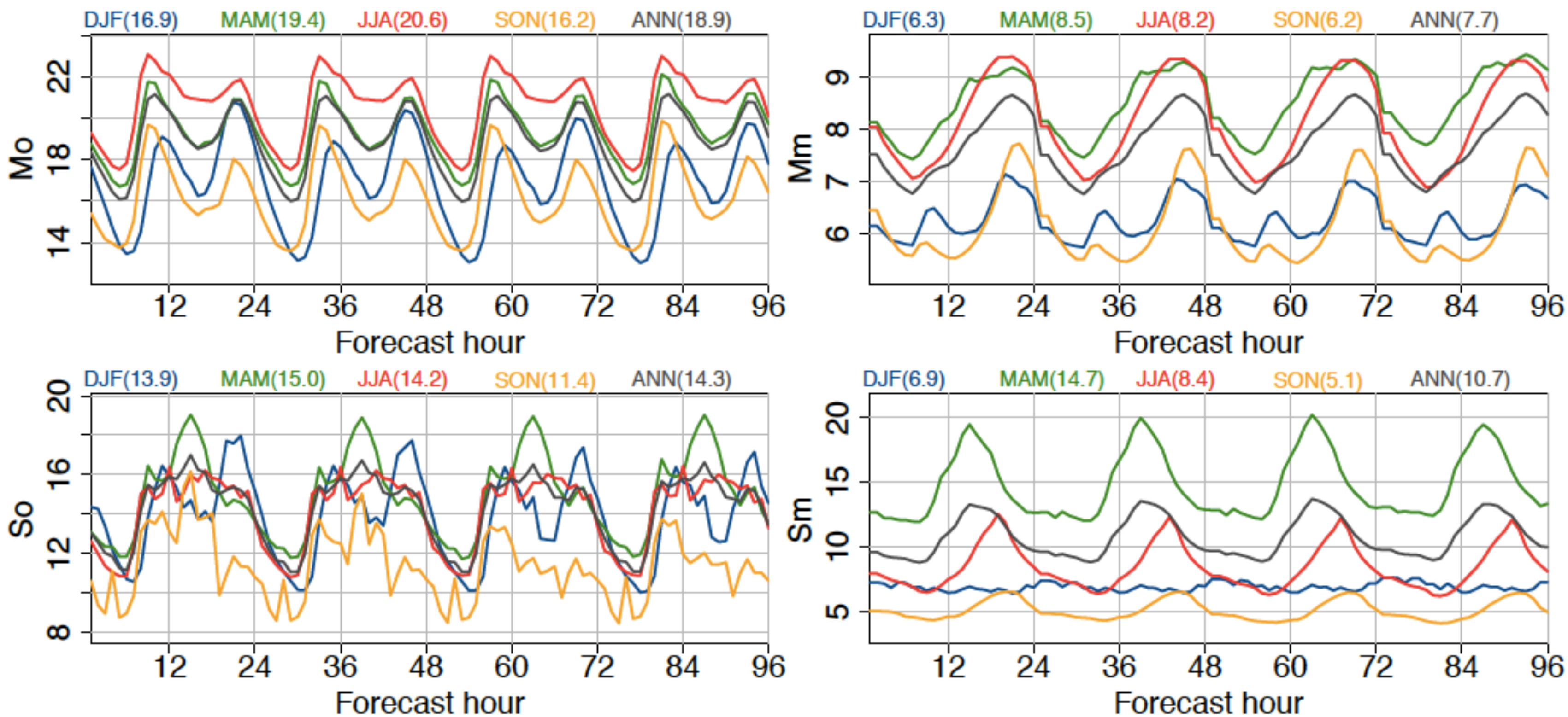
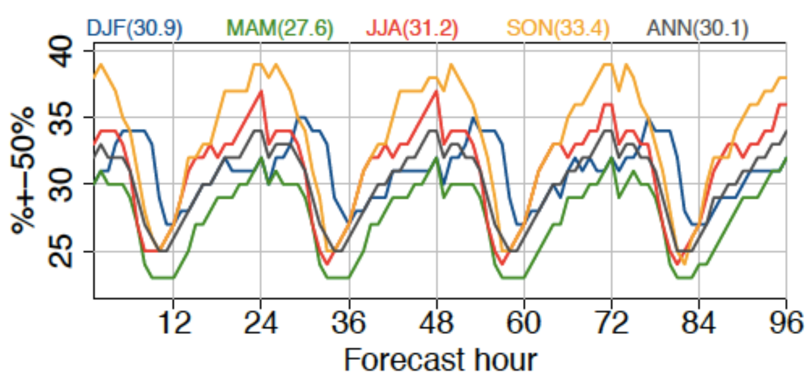
➔ 166 stations

Statistical performance of MONARCH (PM10/IP)





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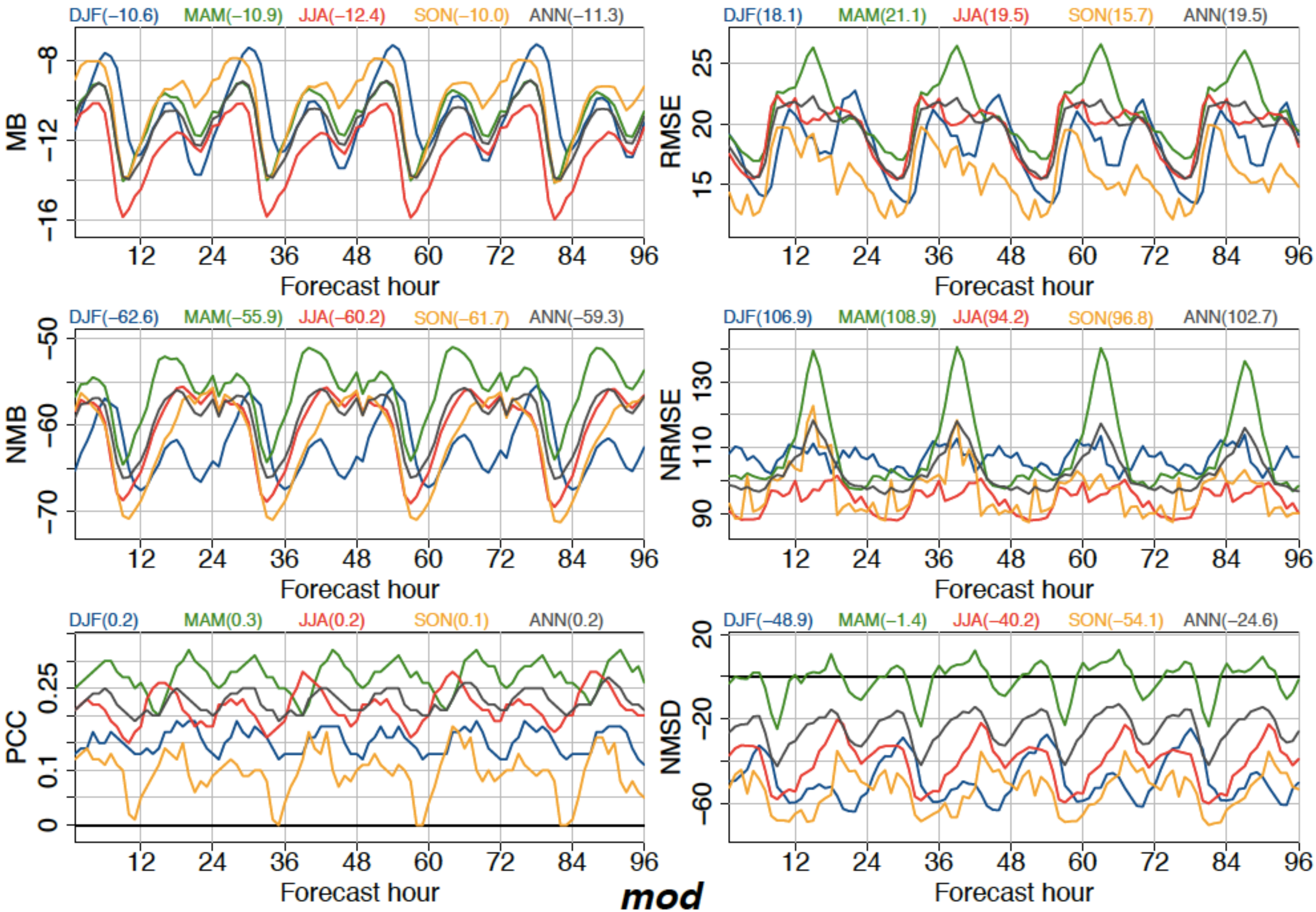
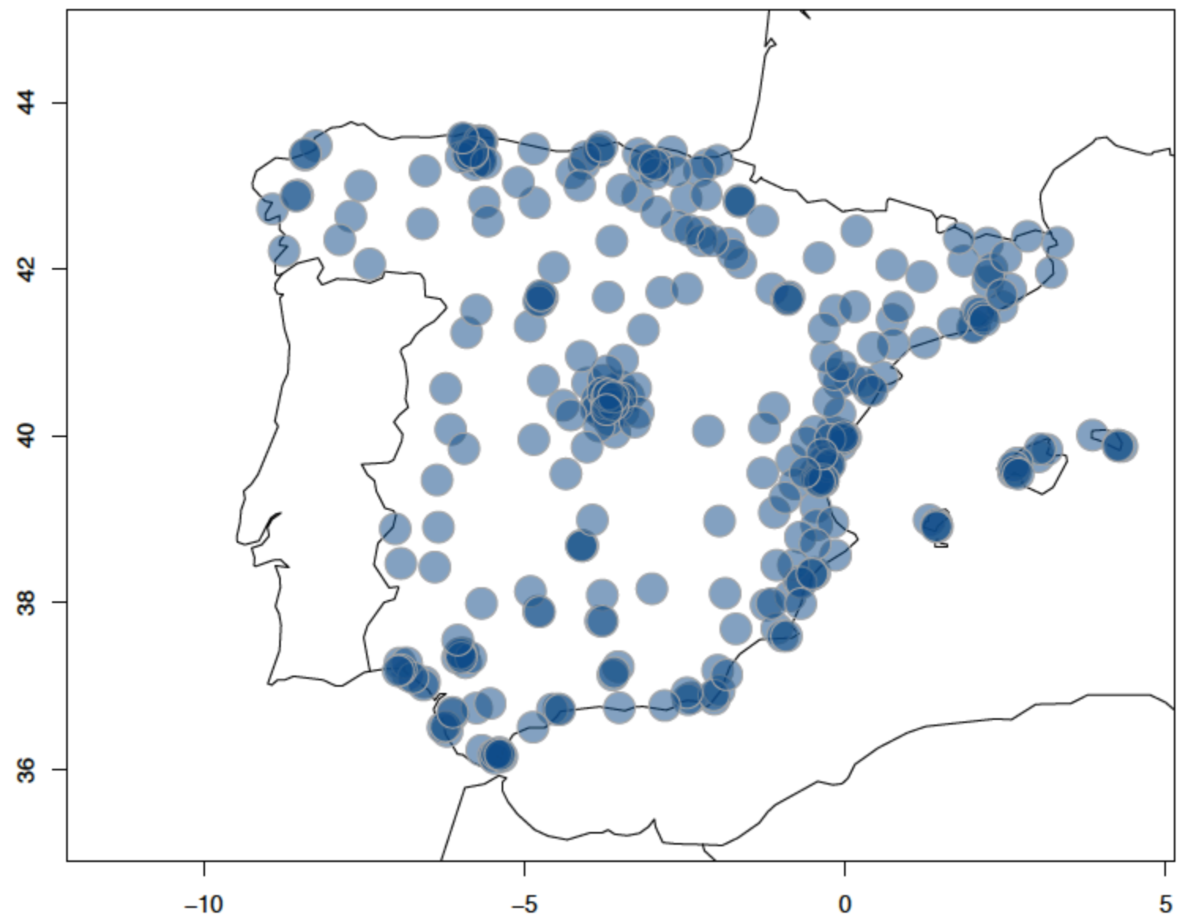
Statistical performance of MONARCH (PM10/IP)

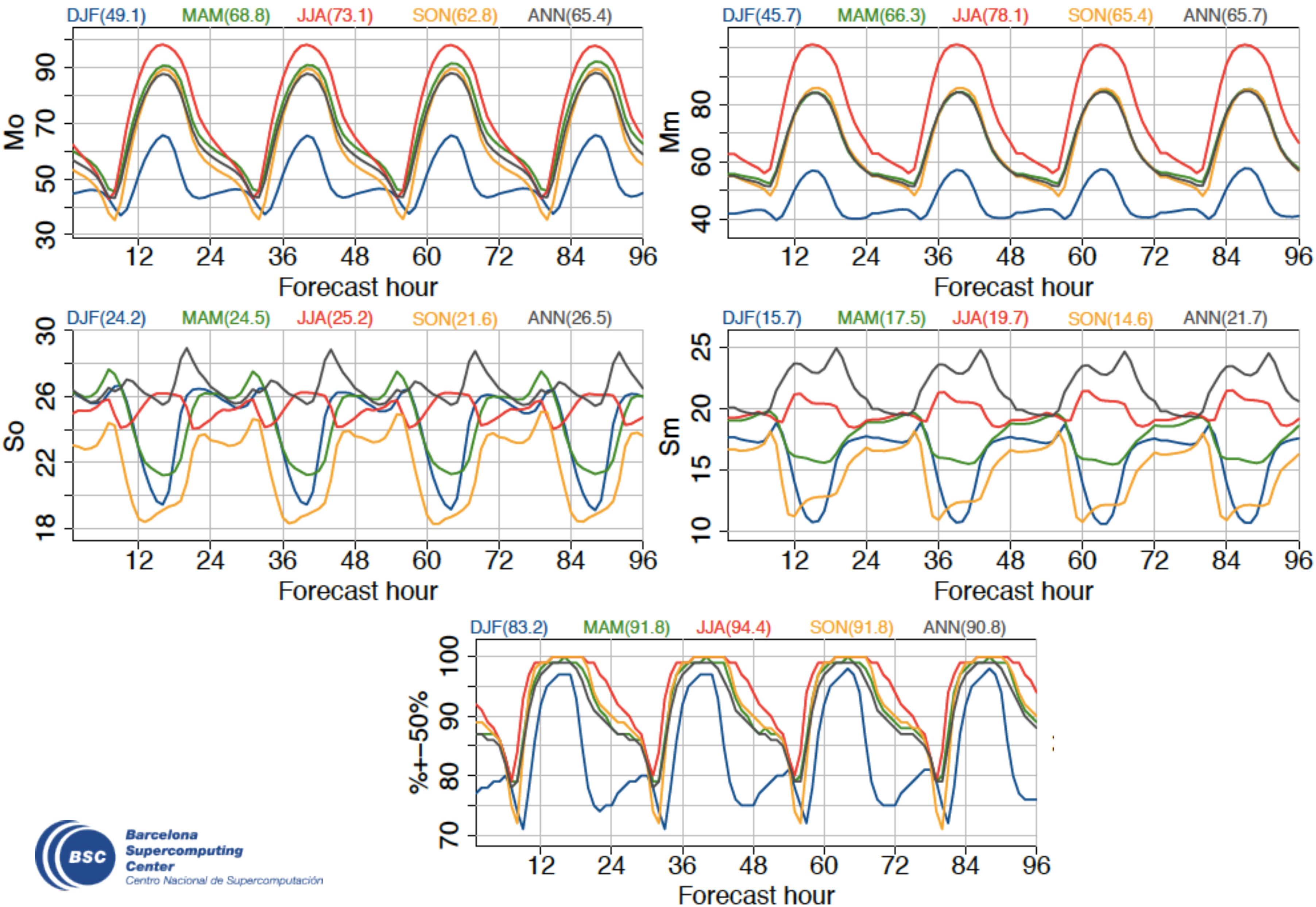


Statistical performance of MONARCH (O3/IP)



➔ 312 stations

Statistical performance of MONARCH (O3/IP)



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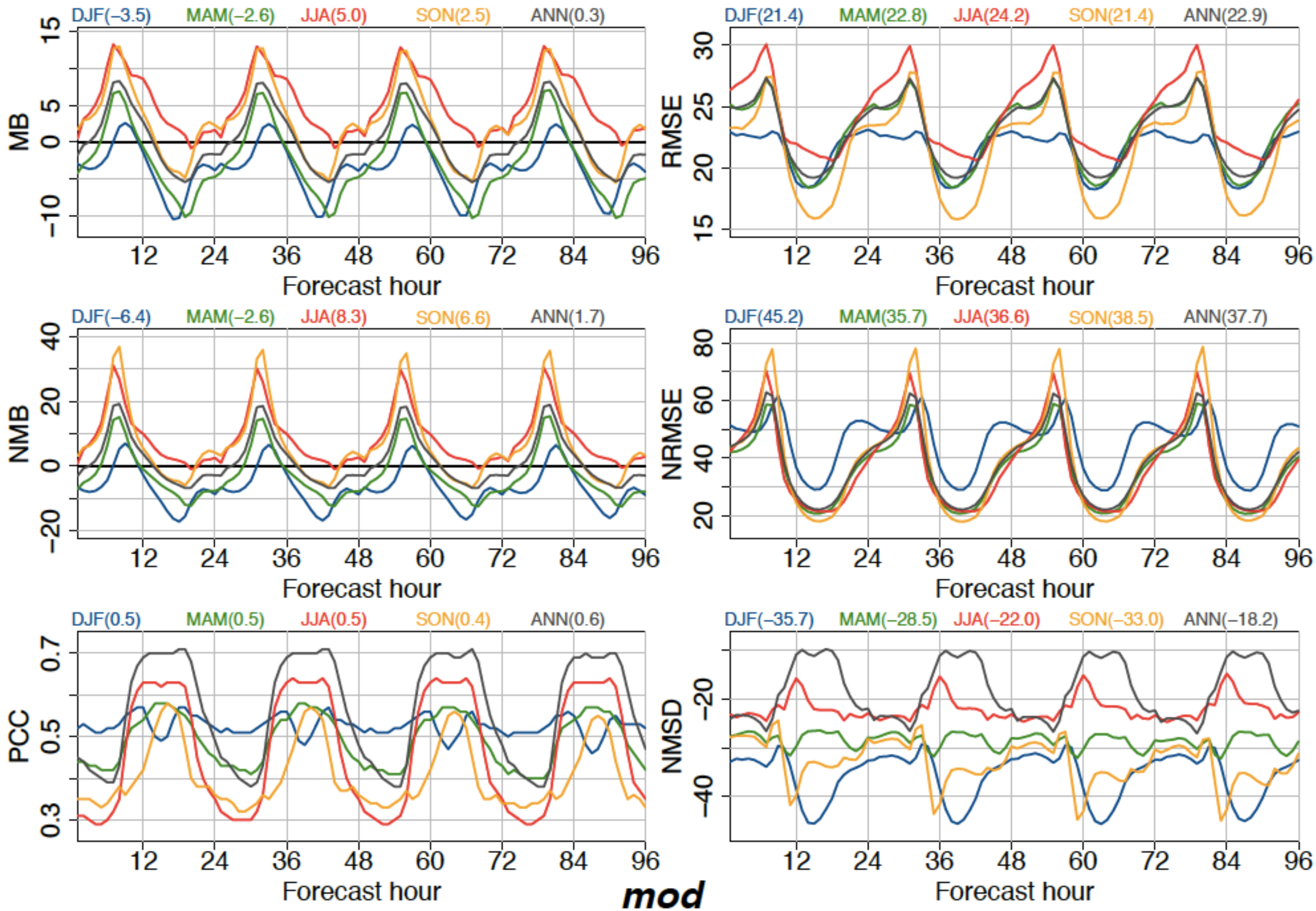
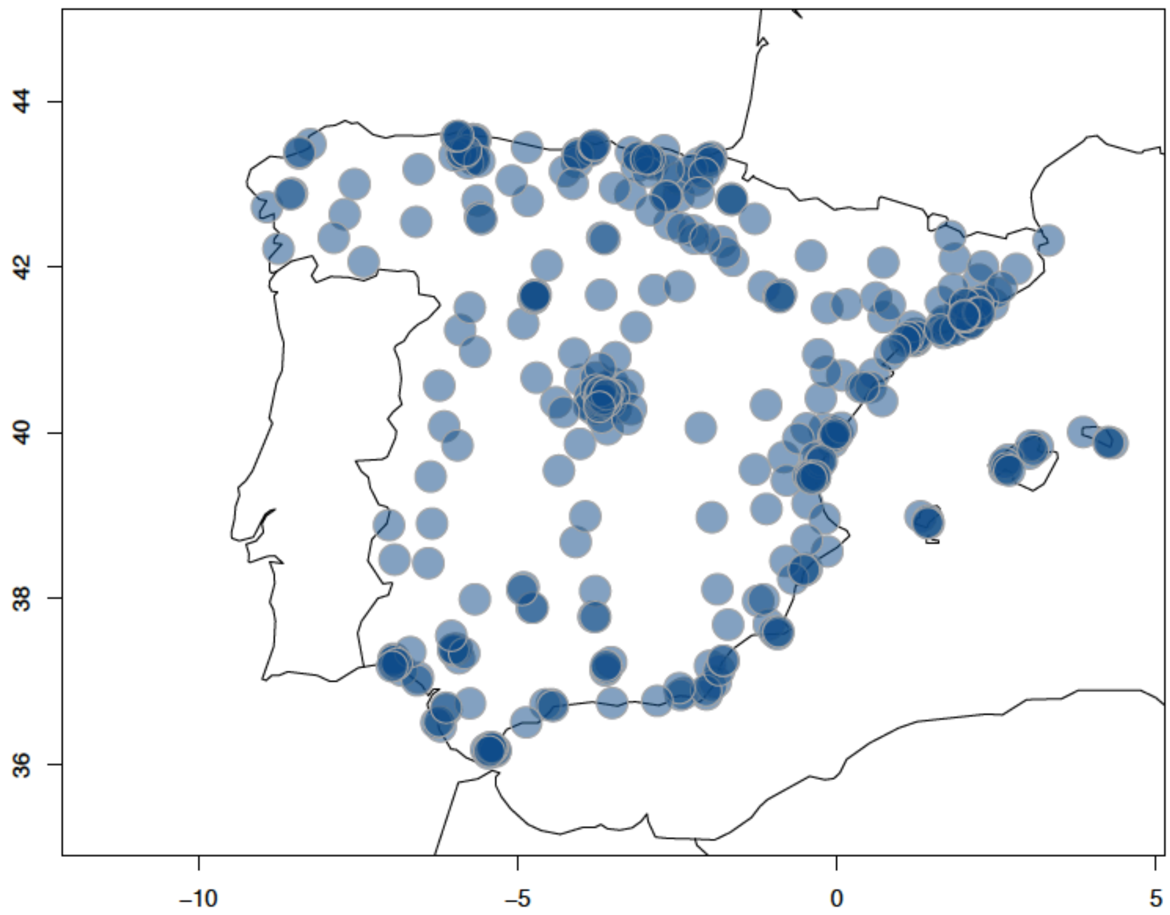
Statistical performance of MONARCH (O3/IP)



Statistical performance of MONARCH (NO2/IP)



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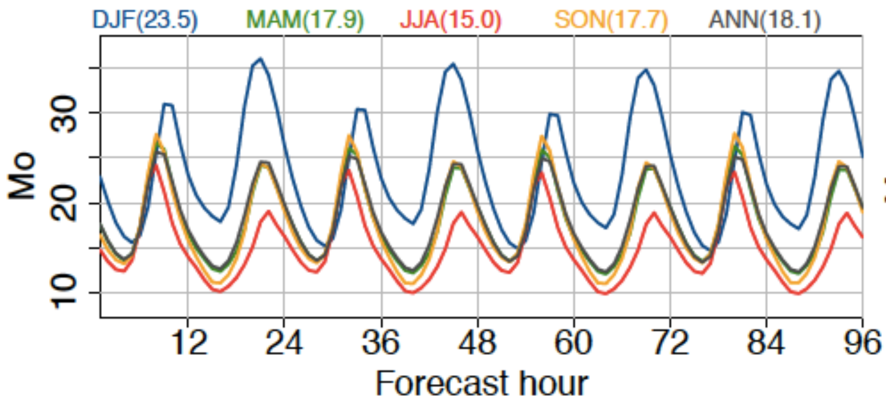
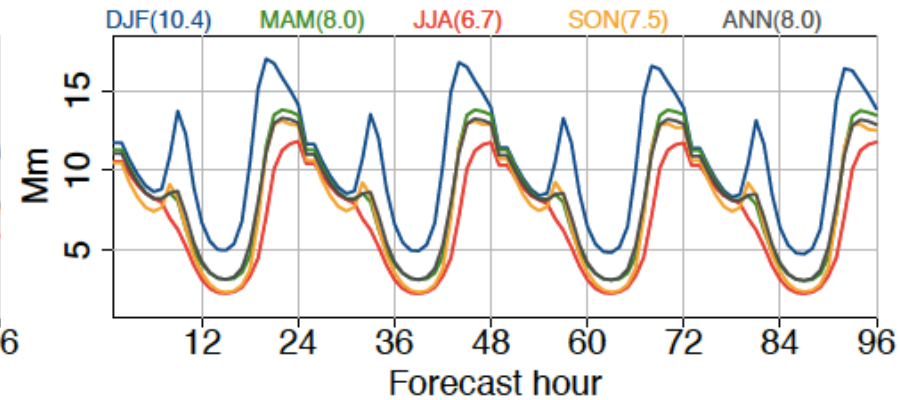
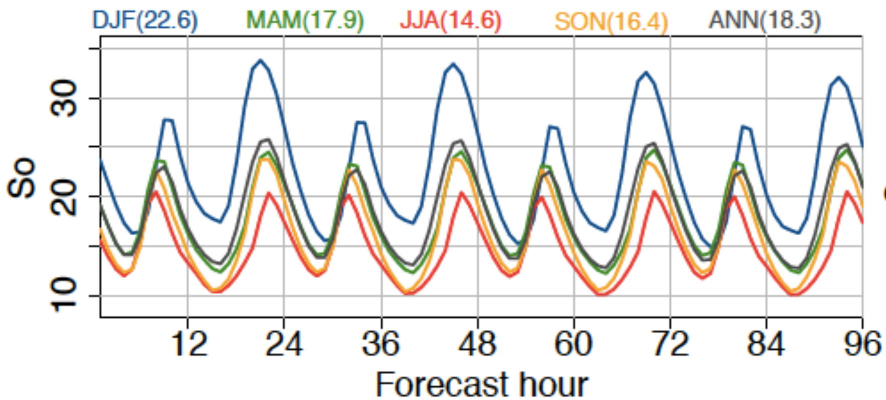
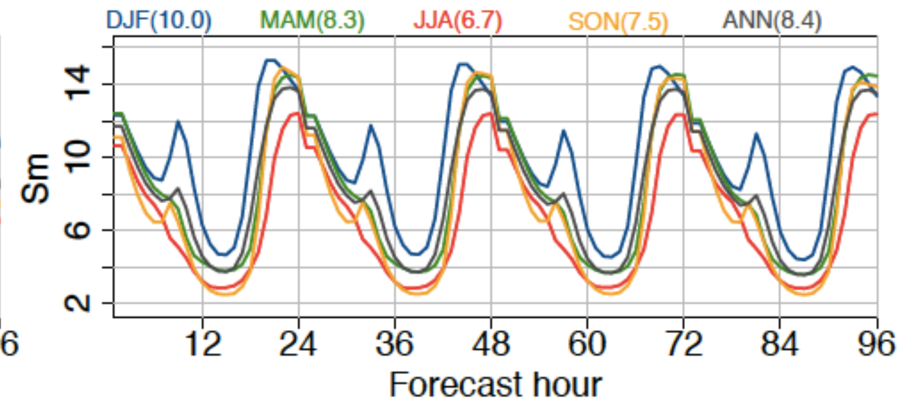
➔ stations

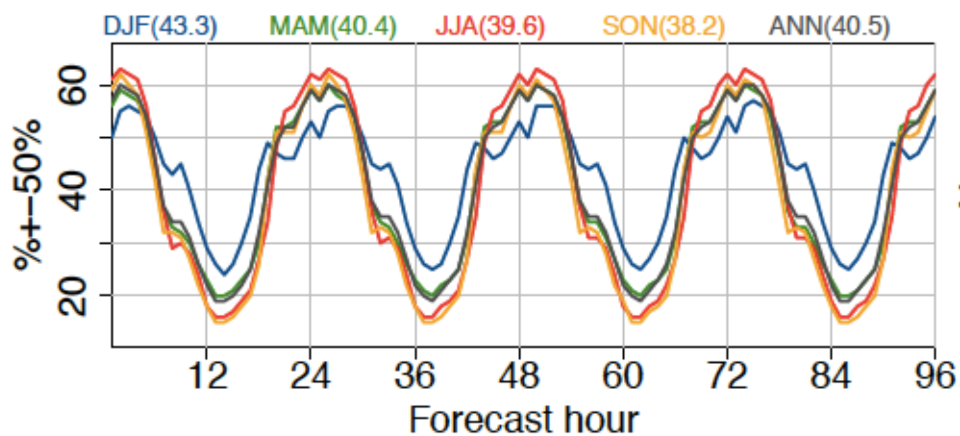
Statistical performance of MONARCH (NO2/IP)











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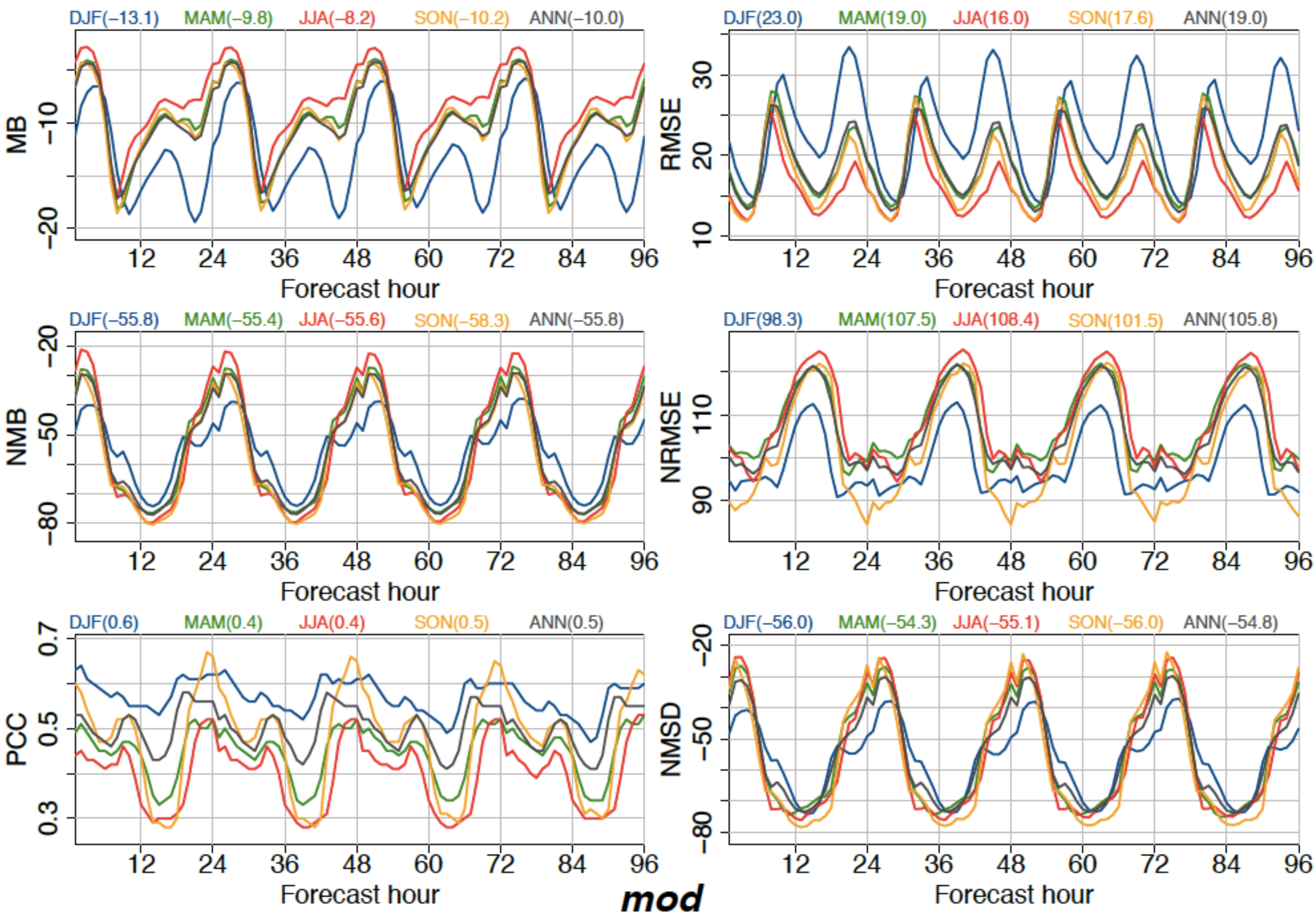
Statistical performance of MONARCH (NO2/IP)



Statistical performance of MONARCH - Overview

Annual statistics (seasonal range when substantial) on IP domain :

	NMB (%)	NRMSE (%)	PCC	NMSD (%)	Ndaily
PM10	-60	103	0.23 (0.10; 0.27)	-25 (-1; -55)	31,000
O3	2 (-3; 8)	38 (36; 45)	0.57 (0.41; 0.53)	-18 (-22; -36)	53,000
NO2	-56	106	0.50 (0.40; 0.57)	-55	65,000

In terms of statistics, no strong differences between station types except for NO2 :
RUR versus URB stations

➔ better NMB (-30% versus -60%)
➔ worst PCC (0.33 versus 0.49)
➔ better NMSD (-33% versus -54%)
➔ worst NRMSE (114% versus 98%)

But statistics can show different diurnal profiles between station types (e.g. O3)

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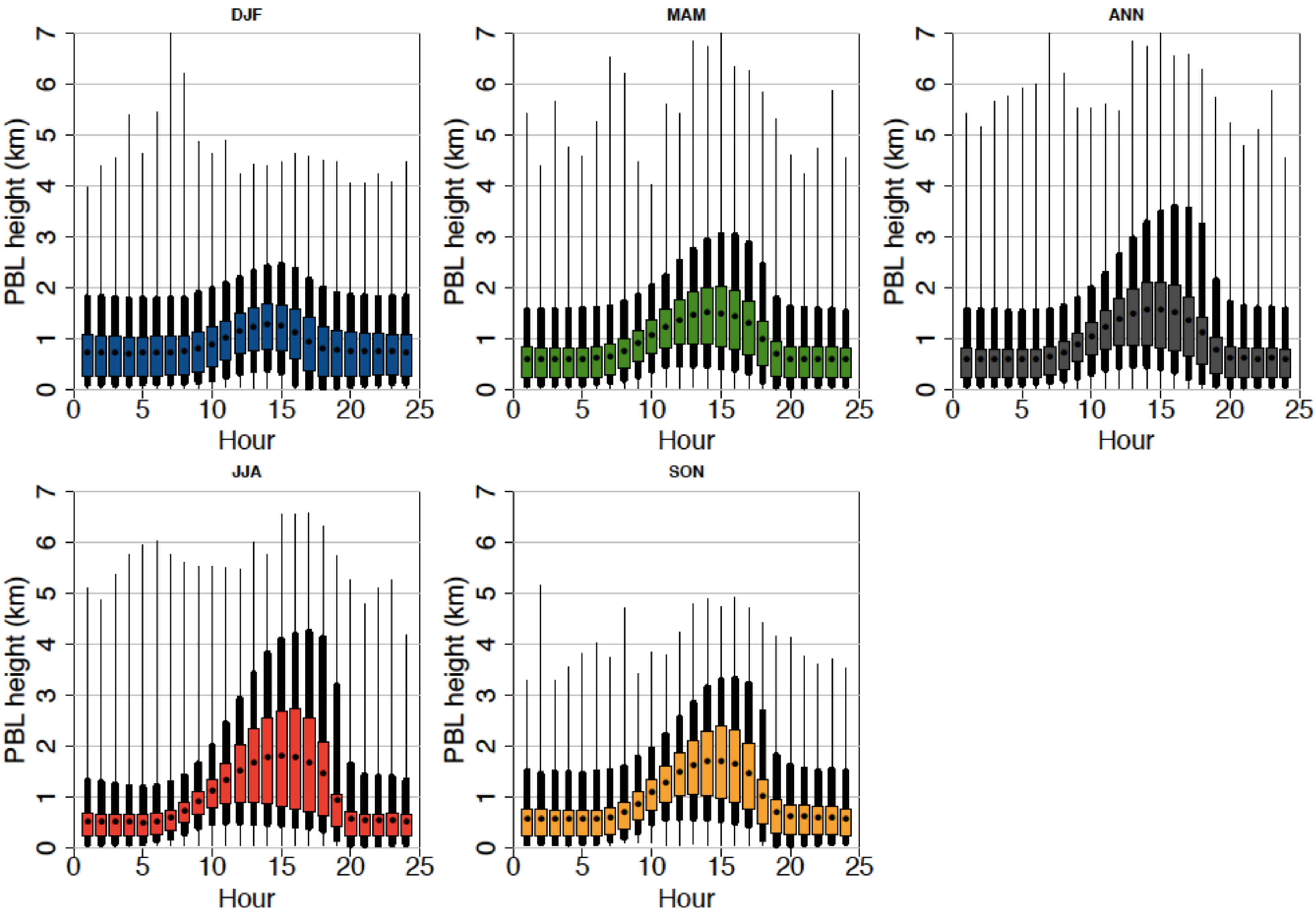
Statistical performance of MONARCH - Overview

- PM10 :
  - PM10 diurnal variability poorly represented
  - Overall strong negative bias (in particular during morning)
  - Strongest errors during morning transition
  - Lowest correlations in winter/fall
- O3 :
  - O3 diurnal variability reasonably well represented for all seasons
  - Overall strong positive bias
  - Strongest errors during morning transition whatever the season (strong positive bias) and late evening in winter (more random errors)
  - Highest (lowest) correlations during afternoon (early morning)
- NO2 :
  - NO2 diurnal variability quite well represented except morning peak (too low) and late evening (too persistent peak)
  - Overall strong negative bias (in particular during morning)
  - Strongest errors during early afternoon
  - Lowest correlations in summer/fall/spring
- All pollutants :
  - Underestimated variability

Statistical performance of MONARCH - Overview

- Strong underestimation of NO_2 during daytime : resolution? emissions? PBL height? vertical mixing? bug?
  - Inconsistent with Badia et al. (2017) : positive bias on rural EMEP stations (e.g. summer, nighttime), despite coarser resolution (1.4°x1°)
  - Check with CAMS50
- More specifically, important issue during morning rush hours : erroneous NO_x and PM emissions (wrong emissions and/or wrong temporal profile) and/or eventually too deep PBL and too coarse resolution
- This leads to strong negative bias on PM (that peaks during morning rush hours) and NO_2 (that peaks in early afternoon) and strong positive bias on O_3 (too low titration by NO?)

PBL height in MONARCH (averaged over IP stations)



MOS correction

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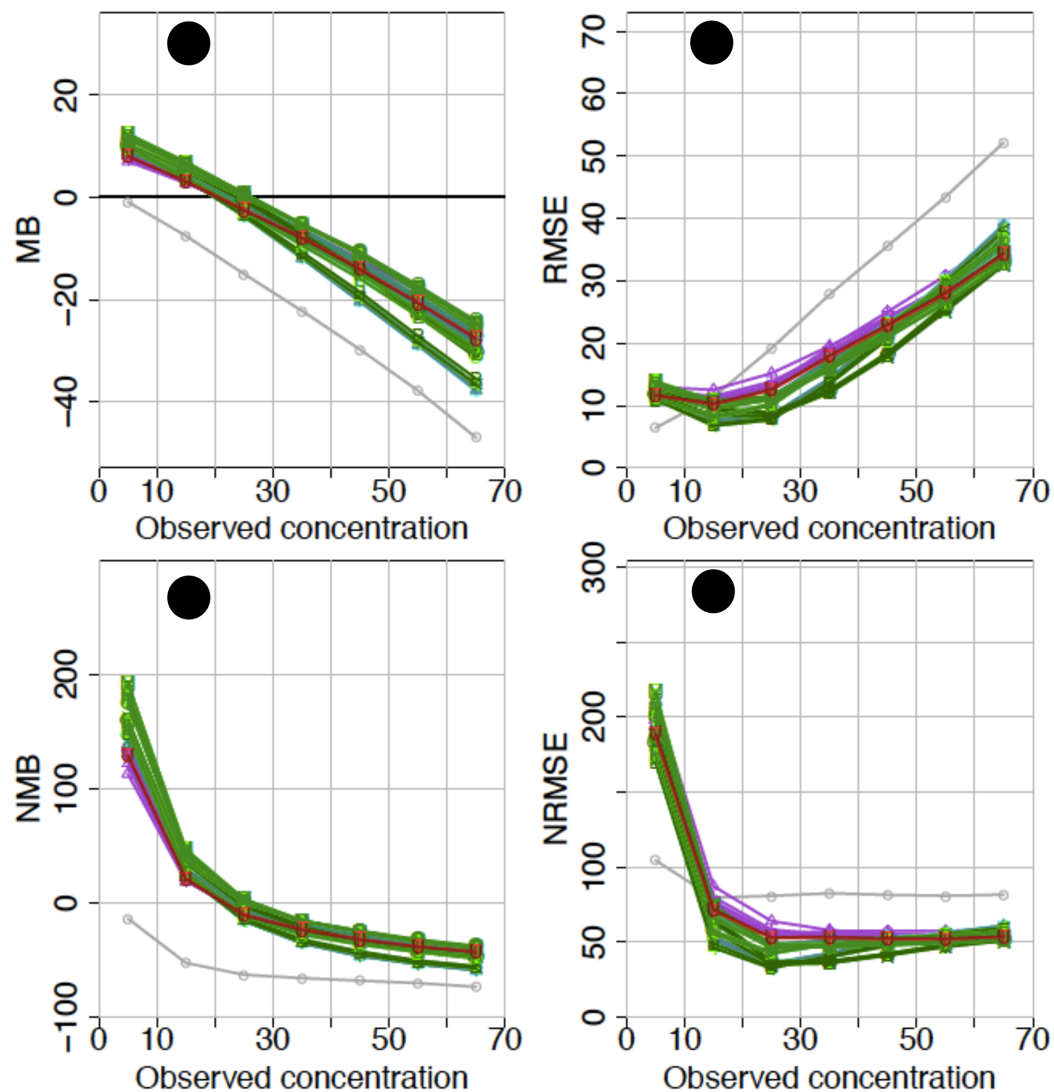
Effect of MOS correction on MONARCH errors

- PM10 : negative bias and error increasing with observed concentration, but quite constant in relative
- MOS correction of PM10 ➔ increase the concentrations to correct the bias, leading to stronger errors in very low concentrations (positive bias) but lower errors elsewhere
- Very similar for NO2



● *Most numerous data*

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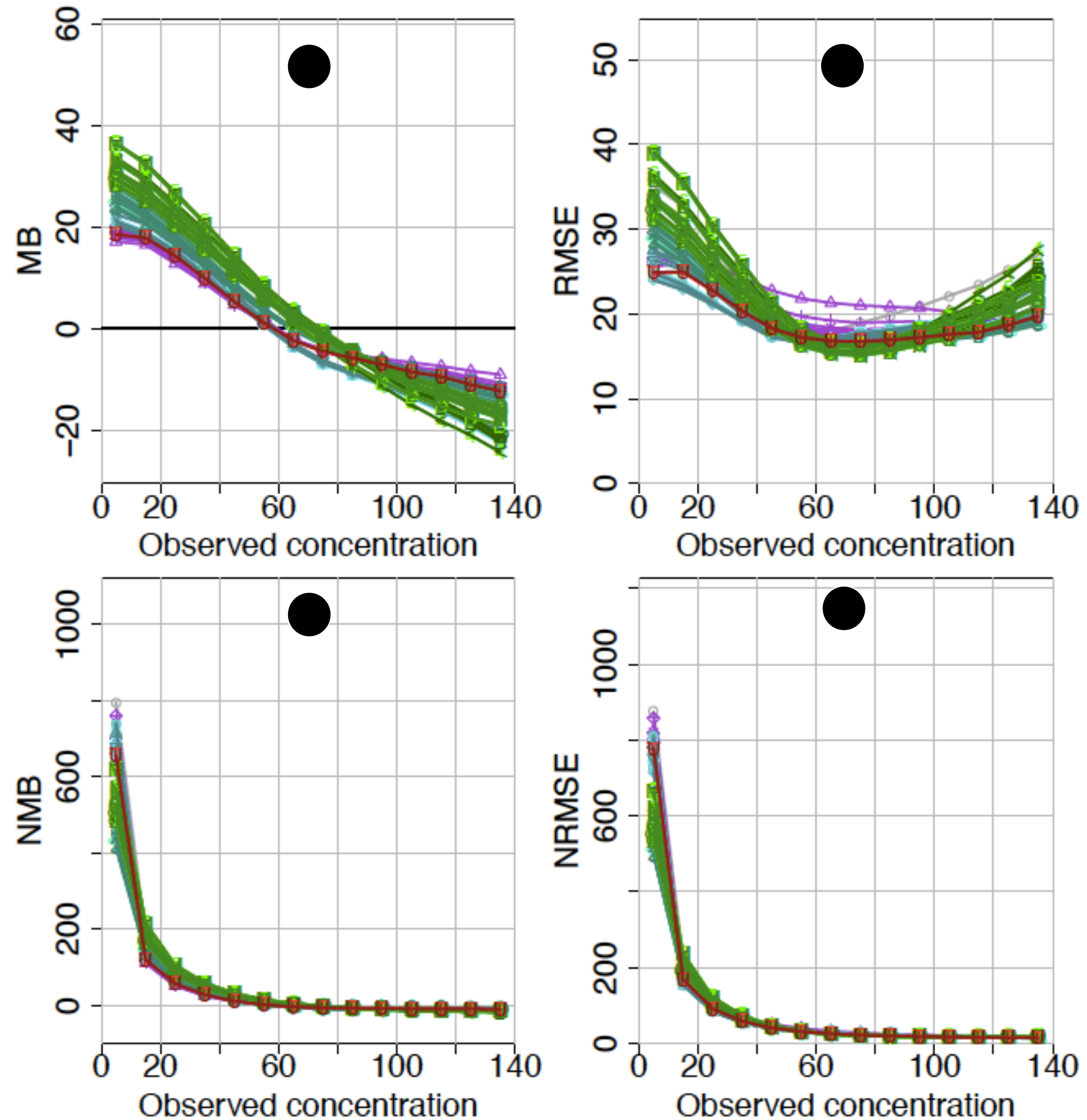
Effect of MOS correction on MONARCH errors

- O3: positive (negative) bias on lower (higher) concentrations
- MOS correction ➔ reduce both negative and positive bias, and usually reduce the error over the whole range of observed concentrations



● *Most numerous data*

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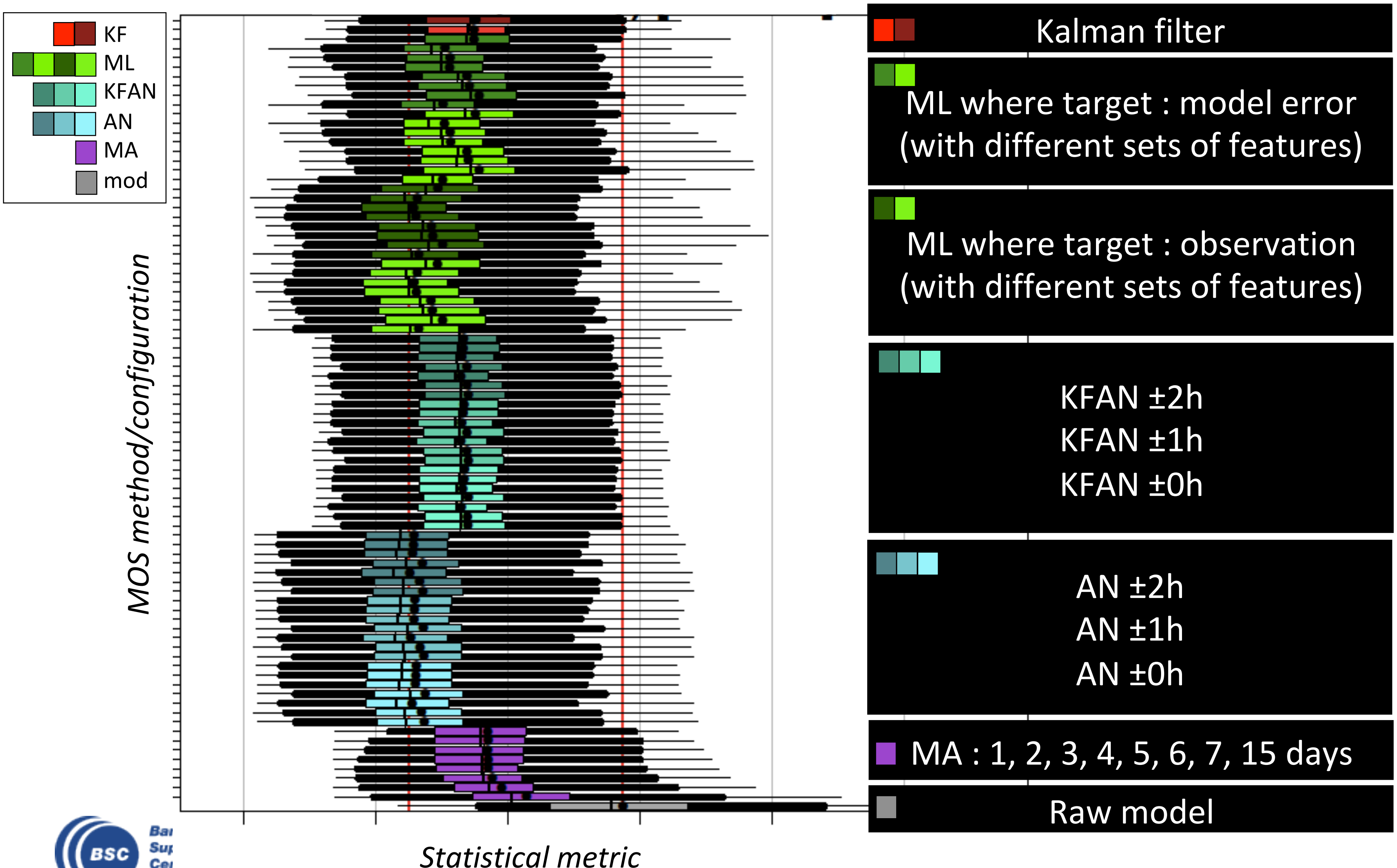
MOS methods and configurations



MOS-ML naming convention

Example for the GBM algorithm :

ml_gbm-<start>-<frequency>-<target>-<config_var>-<config_train>-<bagfraction>

- Start : initial number of days before starting to train ML models
- Frequency : frequency (in days) at which the ML model is updated
- Target : 0 if the target is the observed concentration, 1 if the target is the error (mod-obs)
- Config_var : id of the set of features taken into account
- Config_train : id of the training configuration chosen
- Bagfraction : bag.fraction tuning parameter of the GBM algorithm

Example : ml_gbm-90-30-0-1-1-0.75

➔ training start after 90 days, is updated every 30 days, tries to predict the observed concentration, based on the set of features n°1 (modeled concentration + standard meteorological parameters) and the training configuration n°1 (default), with bag fraction of 75%

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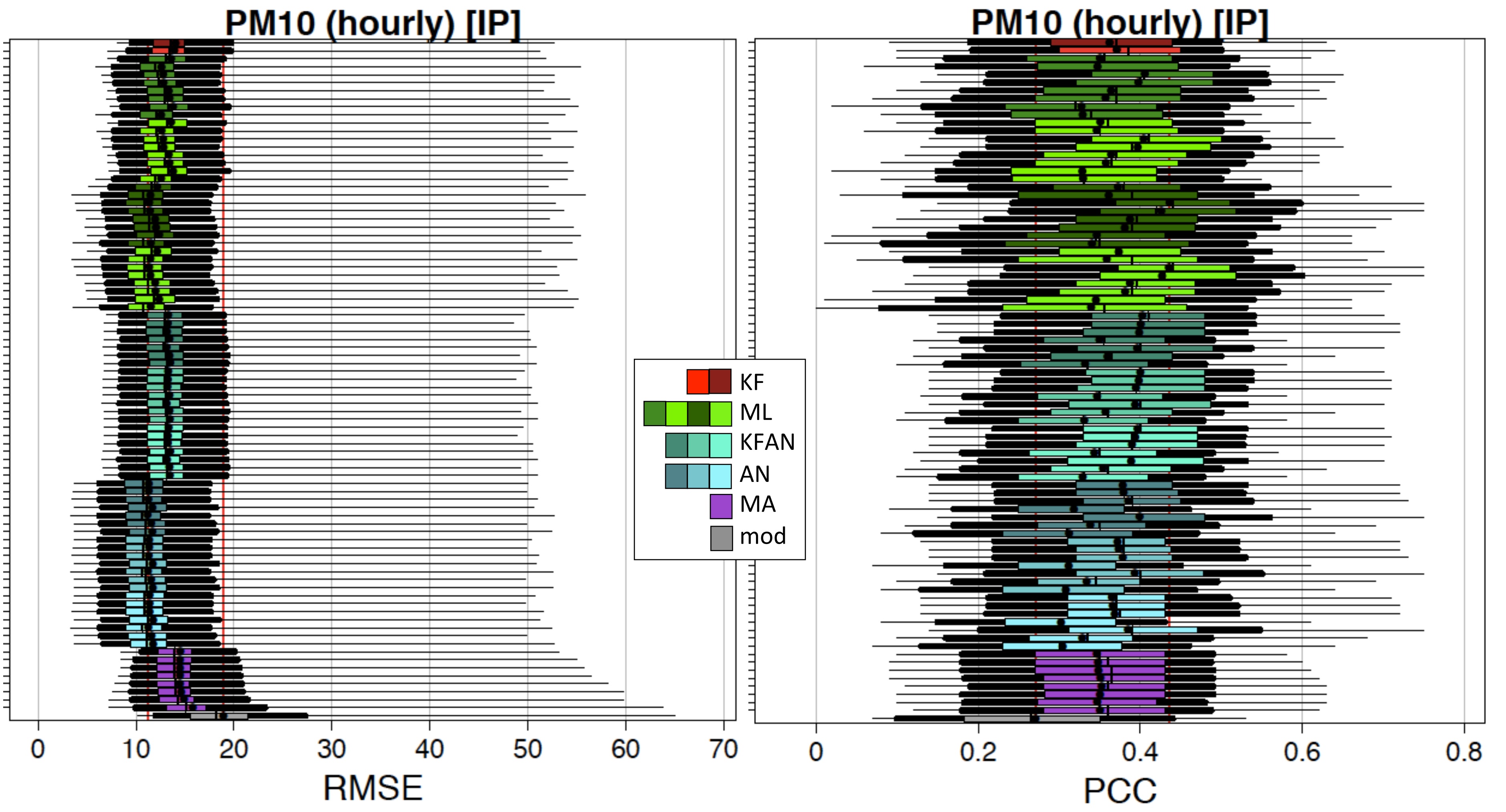
MOS correction on PM10



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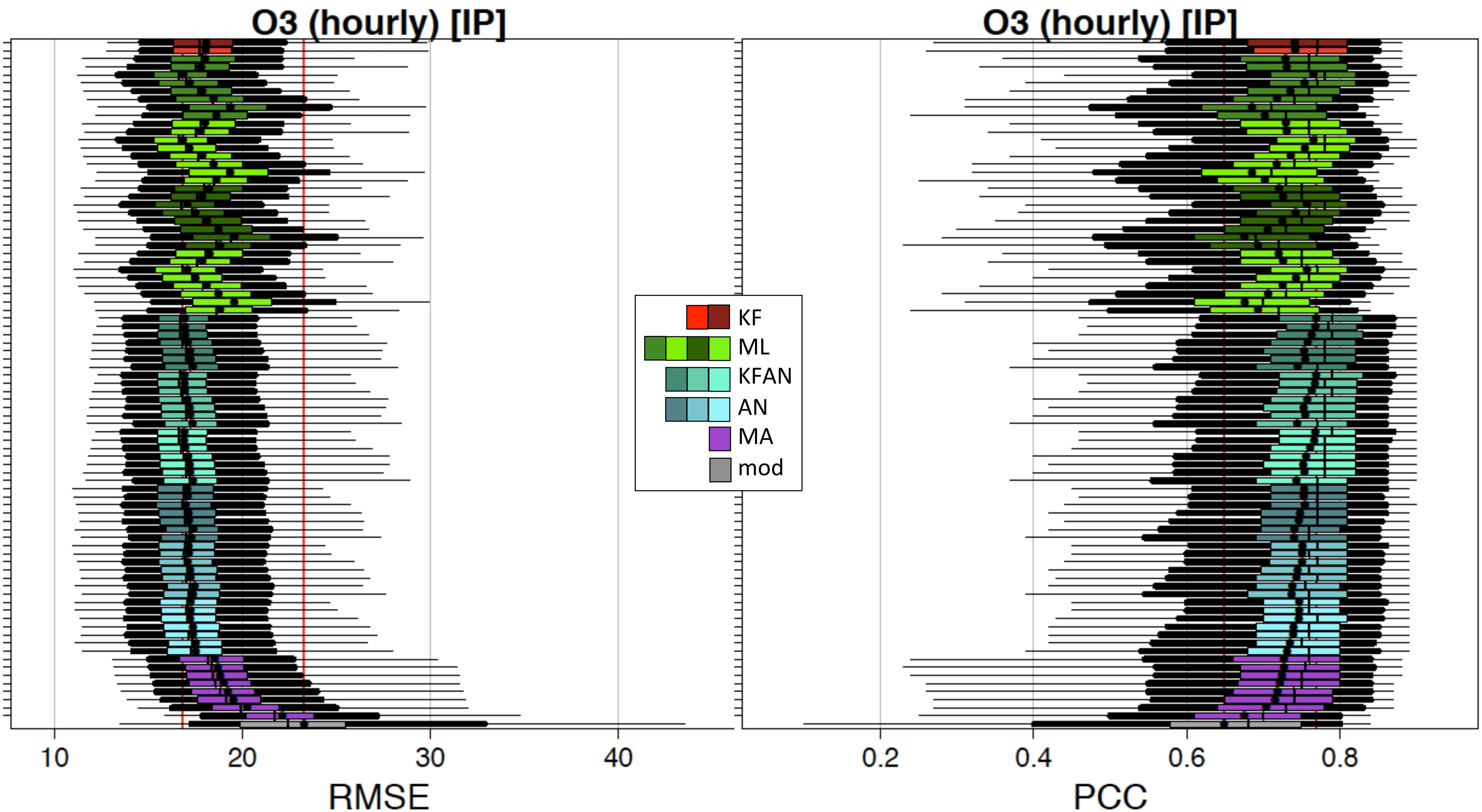
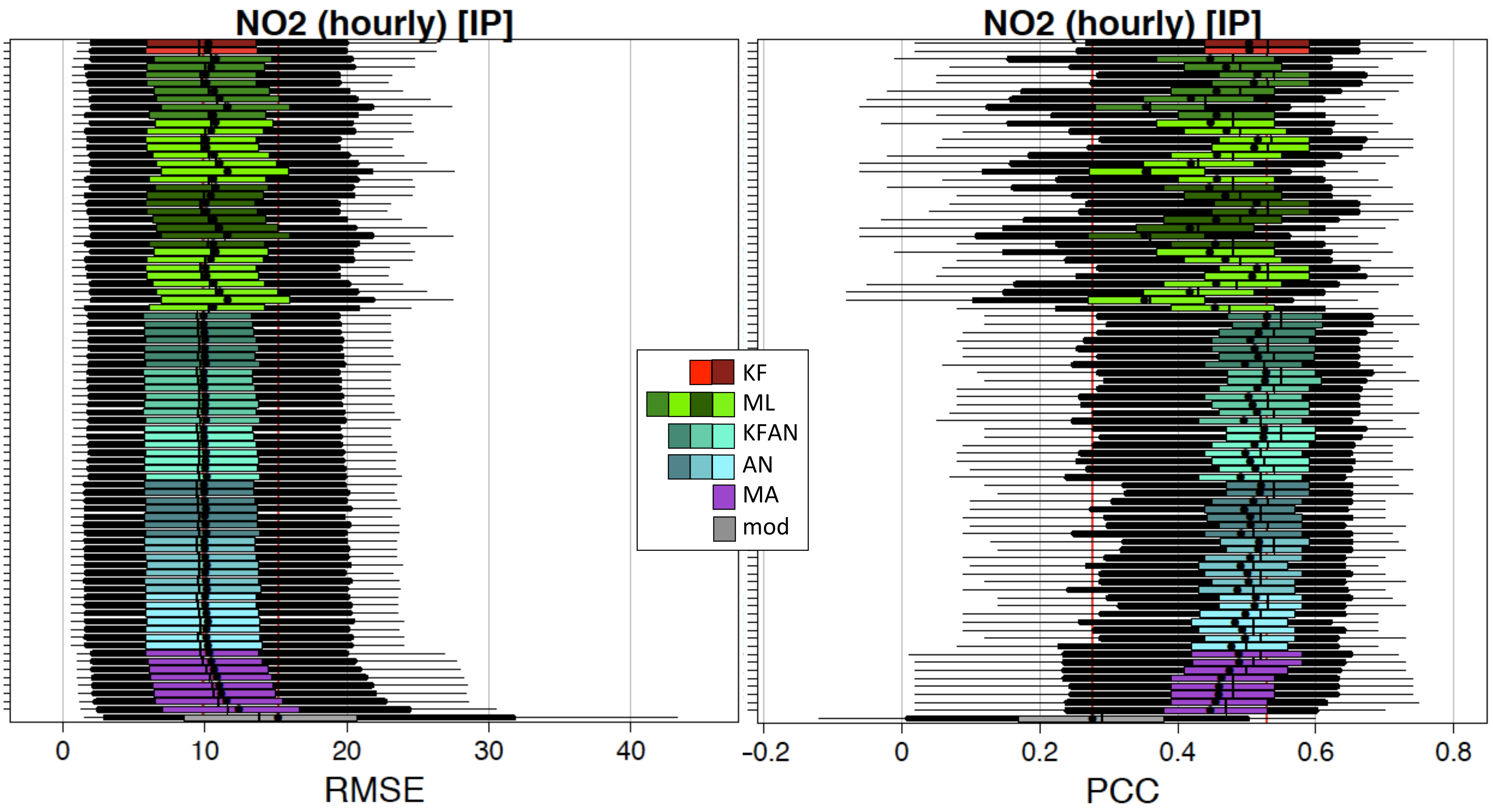
MOS correction on O3



MOS correction on NO2



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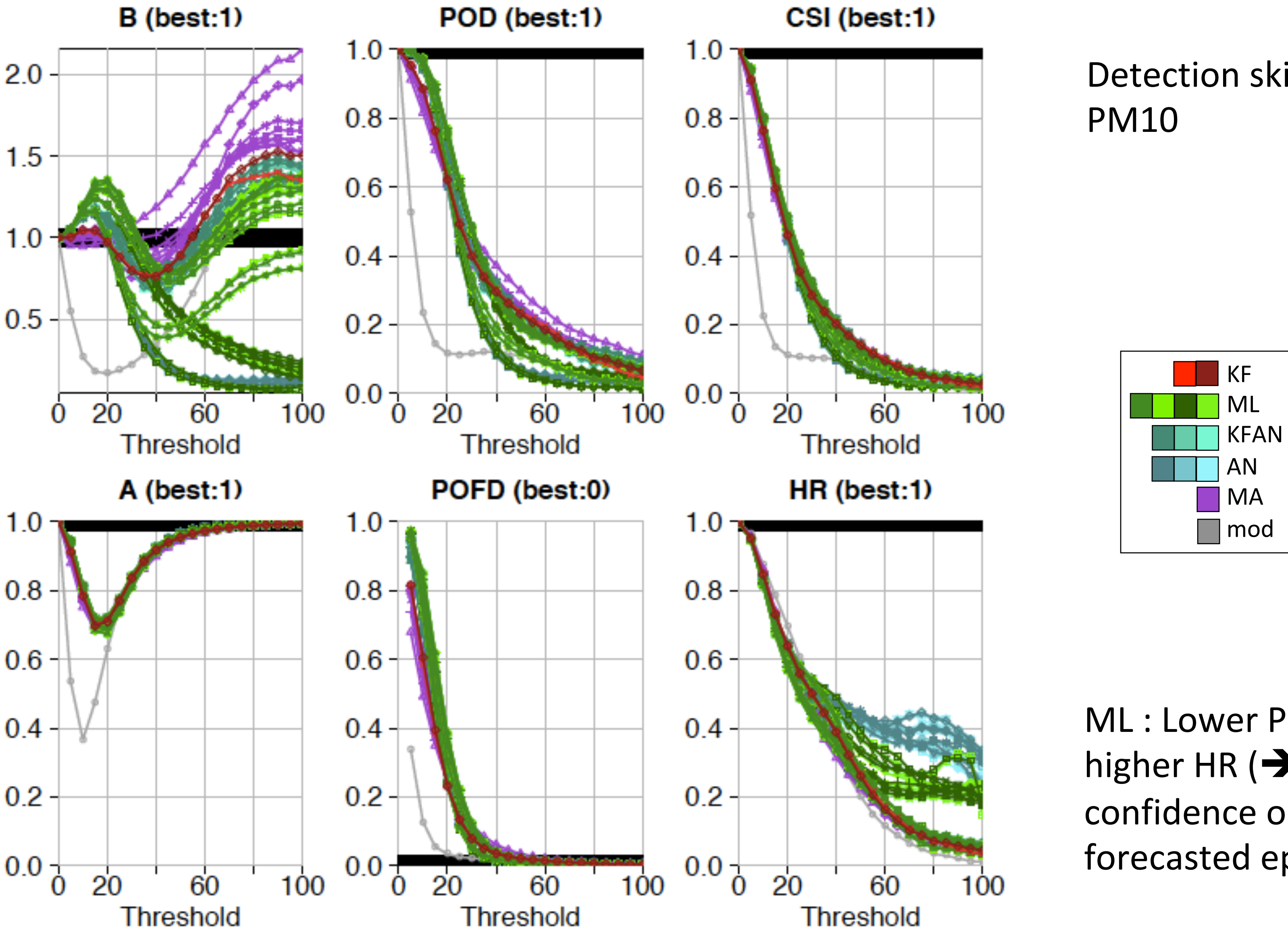
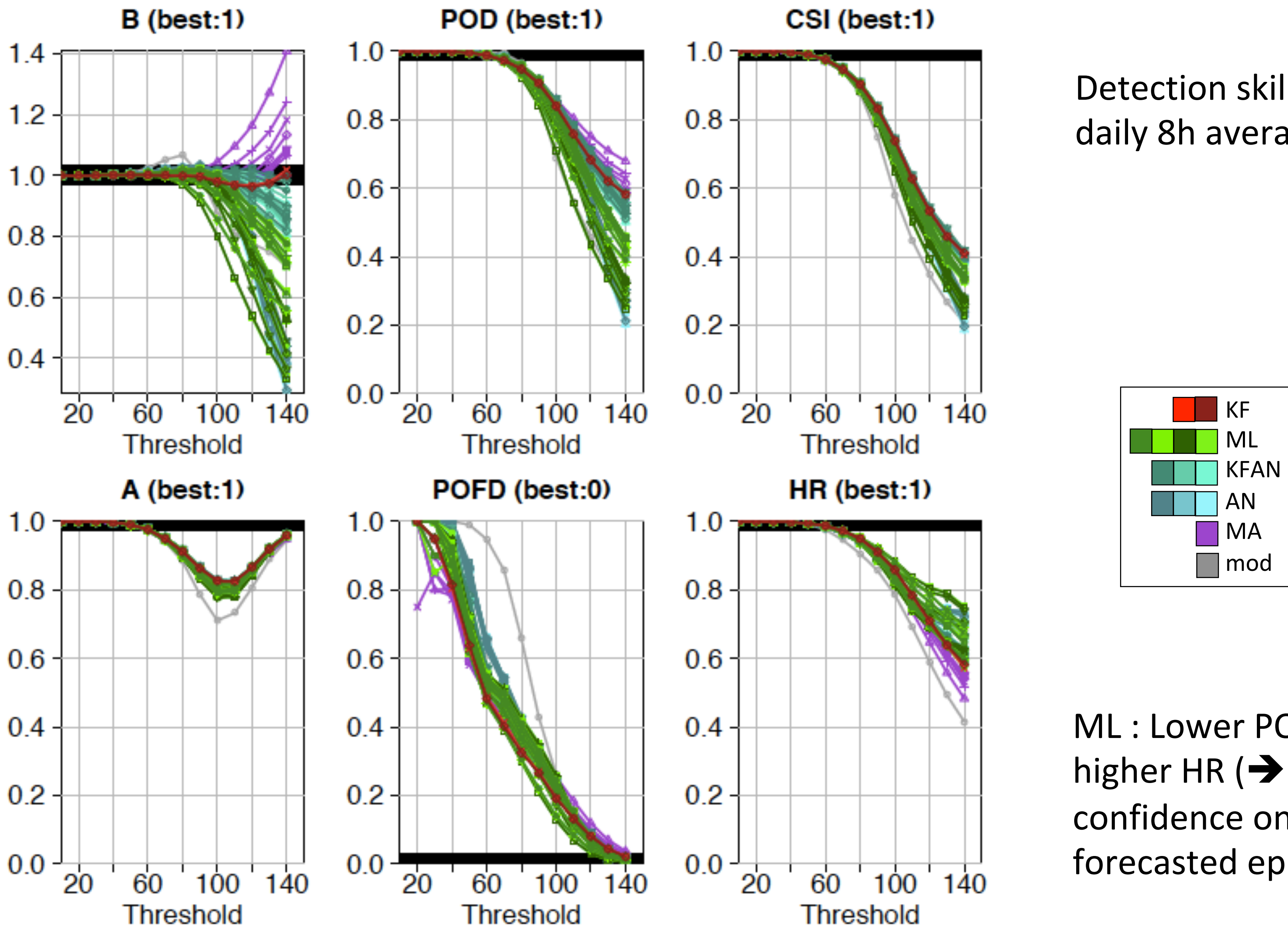
Episode detection



Detection skills – Hourly PM10

ML : Lower POD but higher HR (➔ more confidence on the forecasted episodes)

Episode detection



Detection skills – Max daily 8h average O3

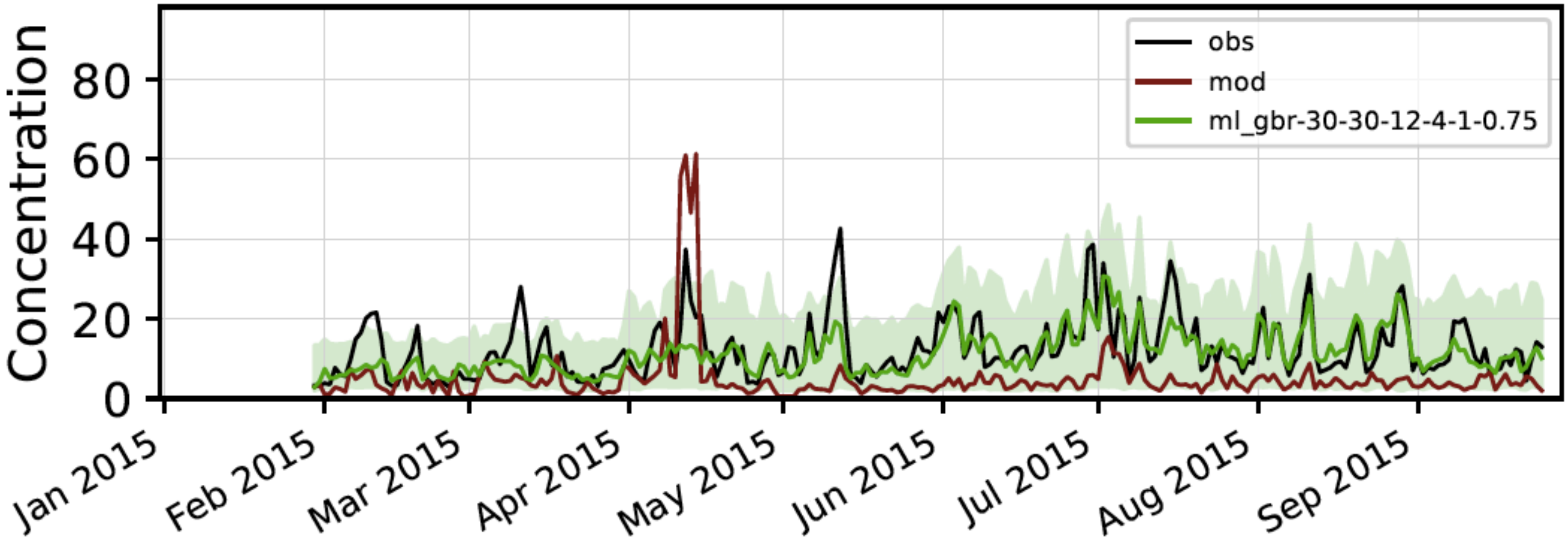
ML : Lower POD but higher HR (➔ more confidence on the forecasted episodes)

Conclusions

- Differences between the MOS methods generally quite consistent from one type of stations to another (URB, SUB, RUR) (not shown)
- Results with traditional MOS methods :
  - KF : reference
  - MA : best improvement with windows larger than 5 days, but lower performance compared
  - AN : often better than KF for both RMSE and PCC (despite very short dataset)
  - KFAN : even better than AN but surprisingly only for O3 and NO2 and not for PM10
- MOS-ML :
  - Often gives the best statistical results (again, despite very short dataset)
  - Tested with different sets of features, best results when many different features are taken into account : *model[day0], mod[day-1], mod[day-2], meteorology, meteorological gradients, hour of the day, error[day-1], error[day-2]*
  - Better results on PM10 when the target is the observed concentrations rather than the model error (no big difference for O3 and NO2)
- But better statistical results does not imply better skills for detecting episodes! MOS methods often smooth the variability, thus reducing the ability to detect extreme concentrations

On-going and planned work

- Run the new python script over all stations
- Investigate the effect of various data preprocessings (e.g. standardization, log-transformation), test other ML algorithms
- Quantile regression to get the prediction intervals (available only for GBM in python)



On-going work

****************************** hourly:

Proportion of observations with 5-95th ML predictions :	77.84% (N=6552 points) (after 2015-01-01)
Proportion of observations with 5-95th ML predictions :	87.40% (N=5808 points) (after 2015-02-01)
Proportion of observations with 5-95th ML predictions :	89.37% (N=5136 points) (after 2015-03-01)
Proportion of observations with 5-95th ML predictions :	89.73% (N=4392 points) (after 2015-04-01)
Proportion of observations with 5-95th ML predictions :	90.55% (N=3672 points) (after 2015-05-01)
Proportion of observations with 5-95th ML predictions :	91.43% (N=2928 points) (after 2015-06-01)
Proportion of observations with 5-95th ML predictions :	89.90% (N=2208 points) (after 2015-07-01)
Proportion of observations with 5-95th ML predictions :	90.44% (N=1464 points) (after 2015-08-01)
Proportion of observations with 5-95th ML predictions :	84.17% (N=720 points) (after 2015-09-01)

****************************** daily:

Proportion of observations with 5-95th ML predictions :	82.05% (N=273 points) (after 2015-01-01)
Proportion of observations with 5-95th ML predictions :	92.15% (N=242 points) (after 2015-02-01)
Proportion of observations with 5-95th ML predictions :	93.93% (N=214 points) (after 2015-03-01)
Proportion of observations with 5-95th ML predictions :	94.54% (N=183 points) (after 2015-04-01)
Proportion of observations with 5-95th ML predictions :	94.77% (N=153 points) (after 2015-05-01)
Proportion of observations with 5-95th ML predictions :	95.90% (N=122 points) (after 2015-06-01)
Proportion of observations with 5-95th ML predictions :	94.57% (N=92 points) (after 2015-07-01)
Proportion of observations with 5-95th ML predictions :	93.44% (N=61 points) (after 2015-08-01)
Proportion of observations with 5-95th ML predictions :	86.67% (N=30 points) (after 2015-09-01)

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EXCELENCIA SEVERO OCHOA

Thank you

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Episode detection metrics

	Event observed	Event not observed
Event forecasted	a	b
Event not forecasted	c	d

- **Error** : ERROR = (b+c)/(a+b+c+d)   complement of **Accuracy** : A=(a+d)/(a+b+c+d)
  - ➔ *How many events or non-events are erroneously classified?*
- **Probability of detection** : POD = a/(a+c)
  - ➔ *How many observed events have been well predicted by the model?*
- **Probability of false detection** : POFD = b/(b+d)
  - ➔ *How many observed non-events are erroneously classified as events by the model?*
- **Hit rate** : HR = a/(a+b)   complement of **False Alarm Ratio** : FAR = b/(a+b)
  - ➔ *Over all events forecasted by the model, how many are indeed observed?*
- **Critical success index** : CSI = a/(a+b+c)
  - ➔ *If we ignore the (numerous) non-events, how many events are correctly detected?*
- **Bias** : B=(a+b)/(a+c)
  - ➔ *Are we forecasting the correct number of events? (no matter when they occur or if the are correct)*

MONARCH alone

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Statistical performance of MONARCH - O3

- URB stations :
  - O3 dynamics reasonably well represented for all seasons
  - Overall strong positive bias
  - Strongest errors during morning transition whatever the season (strong positive bias) and late evening in winter (more random errors)
  - Highest (lowest) correlations during afternoon (early morning)
  - Underestimated variability, in particular during winter/fall afternoon

- RUR stations :
  - Some differences in O3 dynamics, notably in summer
  - Mainly moderate negative biases
  - Idem but different share between random and systematic errors
  - Idem
  - Stronger underestimation of the variability, in particular during night whatever the season and also afternoon in winter/fall

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Statistical performance of MONARCH – PM10

- URB stations :
  - PM10 dynamics poorly represented
  - Overall strong negative bias (in particular during morning)
  - Strongest errors during morning transition
  - Lowest correlations in winter/fall
  - Underestimated variability, in particular during winter/fall, better in spring

- RUR stations :
  - Idem
  - Idem (slightly lower bias)
  - Idem
  - Idem
  - Idem

Statistical performance of MONARCH – NO_2

- URB stations :
  - NO_2 dynamics quite well represented except morning peak (too low) and late evening (too persistent peak)
  - Overall strong negative bias (in particular during morning)
  - Strongest errors during early afternoon
  - Lowest correlations in summer/fall/spring
  - Underestimated variability, in particular during early afternoon

- RUR stations :
  - Idem
  - Idem (slightly lower bias)
  - Idem
  - Idem
  - Idem

Conclusions

- Statistical results in short (at annual scale) :
    - PM10 – URB/RUR : -60% bias, 100-110% error, 0.25 correlation
    - O3 – URB/RUR : ±10% bias, 30-40% error, 0.5-0.6 correlation
    - NO2 – URB : -60% bias, 100% error, 0.5 correlation
      RUR : -30% bias, 110% error, 0.3 correlation
- To be confirmed : maybe underestimated NOx and PM emissions during morning rush hours, which would explain :
    - Underestimated PM
    - Too low nitration of O3 ➔ strong positive bias
    - Too low NO2 and accumulation of this negative bias during morning ➔ strongest negative bias in early morning
    - NB : May also be at least partly due to the dilution in too coarse grid cells, and/or too deep PBL in the morning