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COST Action TD1105

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Dynamic Neural Network Architectures for on field stochastic calibration of indicative low cost air quality sensing systems

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Scientific context and objectives in the Action

- **General Problem statement:**

Multisensors *"On the Field"* Calibration i.e. by using real world data vs. conventional lab recorded data approach
Counteracting sensor issues:
- Cross sensitivity
- Stability
- Slow Response

- **Brief reminder of MoU objectives:**
  - Impacts on WG2 and SIG4

Current research activities of the Partner

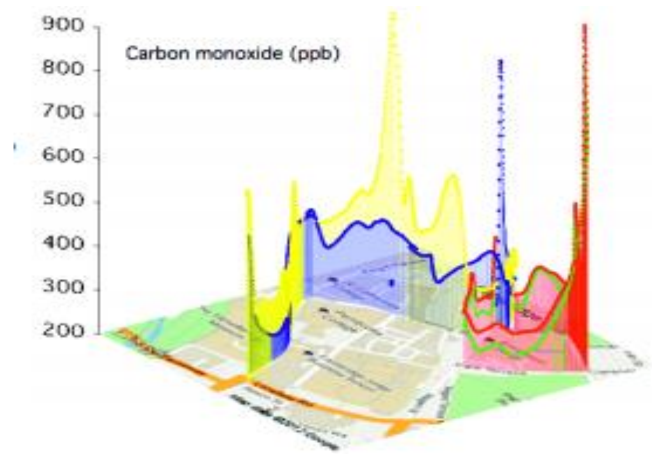
- Brief list of ongoing research topics of the Partner:
  - High Speed dynamic calibration for mobile and pervasive fixed deployments
  - Aveiro Data Processing with Machine Learning approach
  - Machine learning techniques effectiveness comparison
  - Cooperative Air quality monitoring systems

Dynamic calibration for mobile/pervasive deployments

Calibration law State of the art: Use of static neural networks for on the field calibration of air quality multisensors [De Vito et al. 2008, Spinelle et al. 2013-2014]

Could Underperform under New Challenges issued by Mobile and/or pervasive deployments, Robotic applications (source identification), etc:

- – A timely response become paramount for precise and accurate assements
- – … but sensors have their own response dynamic that may results in slow (and hence inaccurate) response



What is the influence of exposure to rapidly changing concentrations?

May Dynamic machine learning approach help in reducing errors?

Machine Learning Calibration Problem (in brief)

Find:

$$Y' = f(sens_1(t_k),\ sens_2(t_k),\ sens_3(t_k), ---,\ sens_n(t_k))$$

where Y' is a single gas true concentration (Y) estimator and $sens_i(t_k)$ is the response of the i sensor at time instant t_k

- Non parametric, Discriminative paradigm
- Learning by Example (Sensor Responses, True Concentrations)
- Hyperparameters to be optimized
- Known to exploit cross sensitivities, robust to outliers
- Seems to provide «best of the show» performance with on field recorded data

Moving to a dynamic paradigm will involve the use of ***time dependant*** features "capturing" sensor dynamics: $Feat_k = g(sens_i(t_{k, k-1, k-2, \ldots, k-s}))$ possibly exploiting past estimations.

The dataset under analysis

This deployment has been carried out by consortium lead by CAS@University of Cambridge

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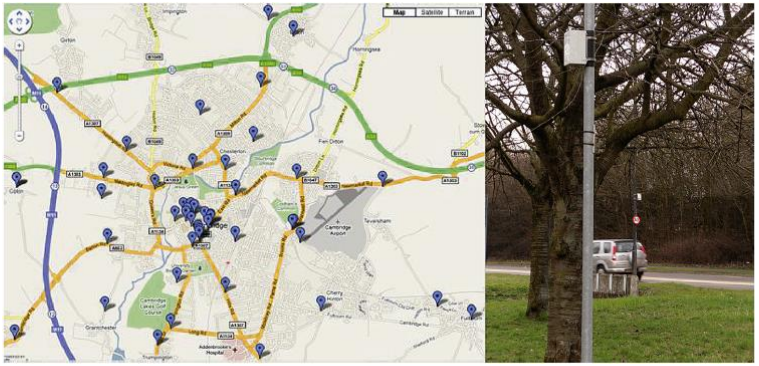


- **More than 30 SNAq stations**
- **Each SNAq station is equipped with at least**
  NO_2, NO, O_3 EC sensors + RH, T
- **Wind speed and direction and a OPC complete the sensor array.**

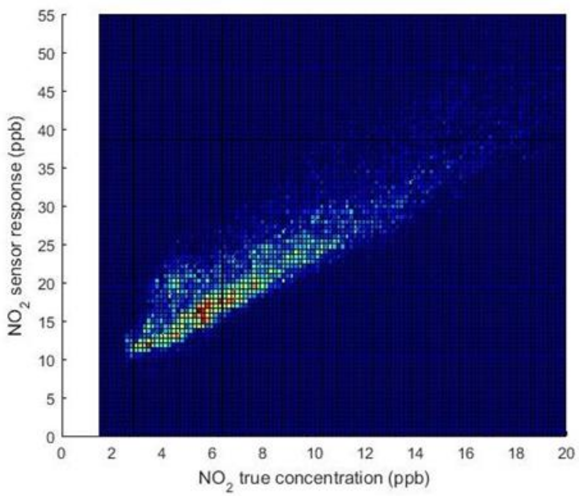
Known cross interference from T and RH (all sensors). O_3 is known to induce strong response in NO_2 targeted EC sensor.

We select the «Roof» station located on the roof of the Chemistry Dept. co-located with a reference chemiluminescence analyzer.
Ts= 20 sec, GT Ts=60sec

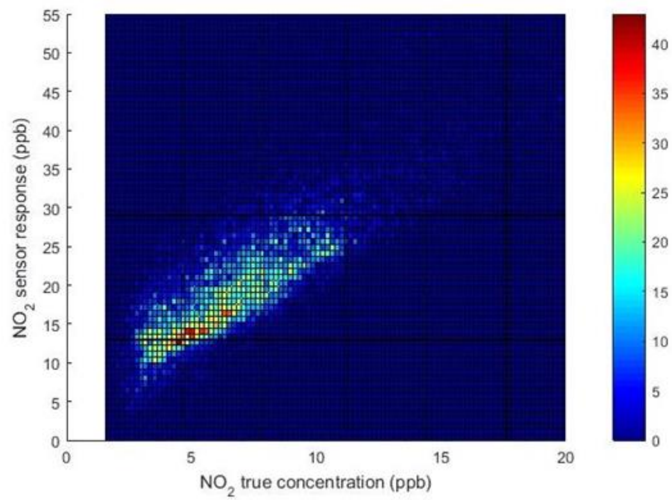
A time series including data sampled during 6 weeks form May to June 2014 has been extracted with a total number of more than 50k samples.
We use a gray box approach with a preprocessing step that subtracts T cross sensitivity effect (datasheet).

Ref.:Mead M.I. et al., The use of EC sensors for monitoring urban air quality in low cost, high density network. Atm. Env., 70, 2013

NO2: correlation with preprocessed data

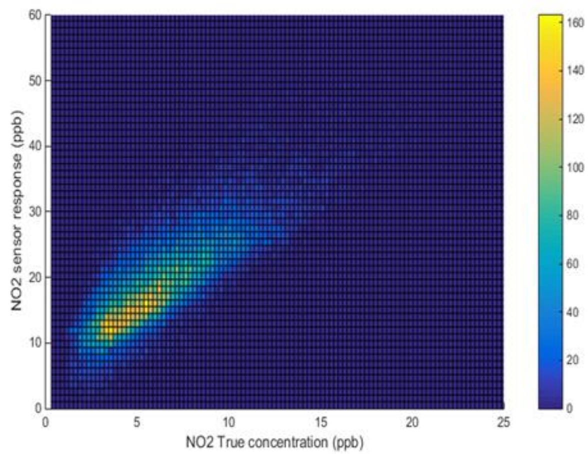


1st Week



2nd Week

Nice Agreement with significant bias.

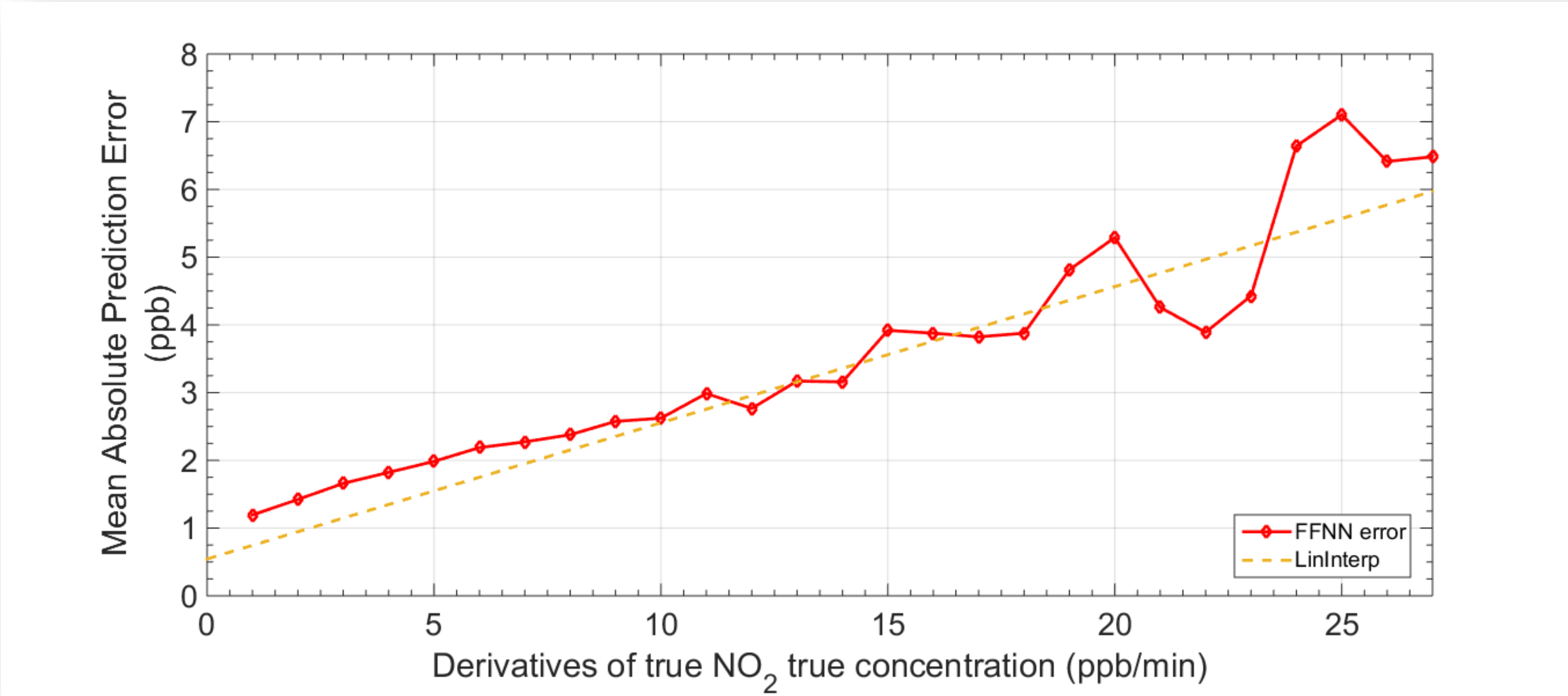


3°+4° Week

Performance are getting worser, due to concept and sensors drift…

NO2: correlation with preprocessed data

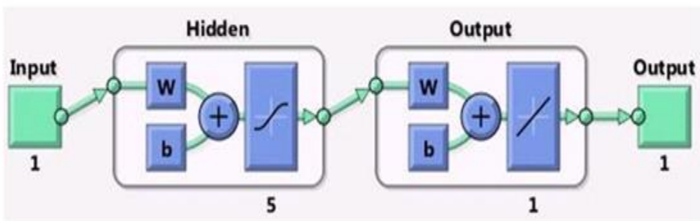
…Moreover, static state of the art approaches shows decaying performances when true concentration changes quickly



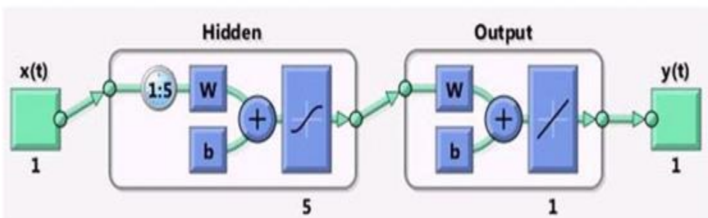
Faster variation induces higher estimation errors!
Can Dynamic Neural Network help to recover?

Focus on Dynamic Neural Architectures

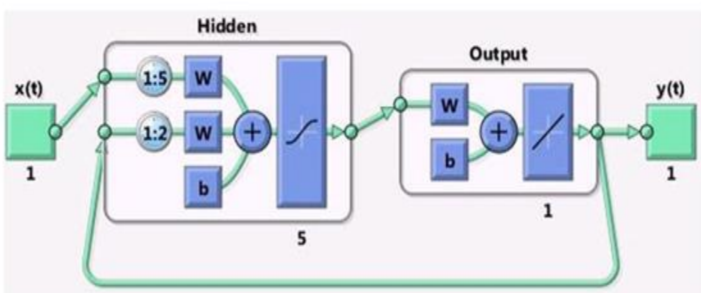
- We compared results obtained by 3 architectures:



FFNN : a static BPNN fed with sensor responses.
Hyperparameters: # of hidden neurons.

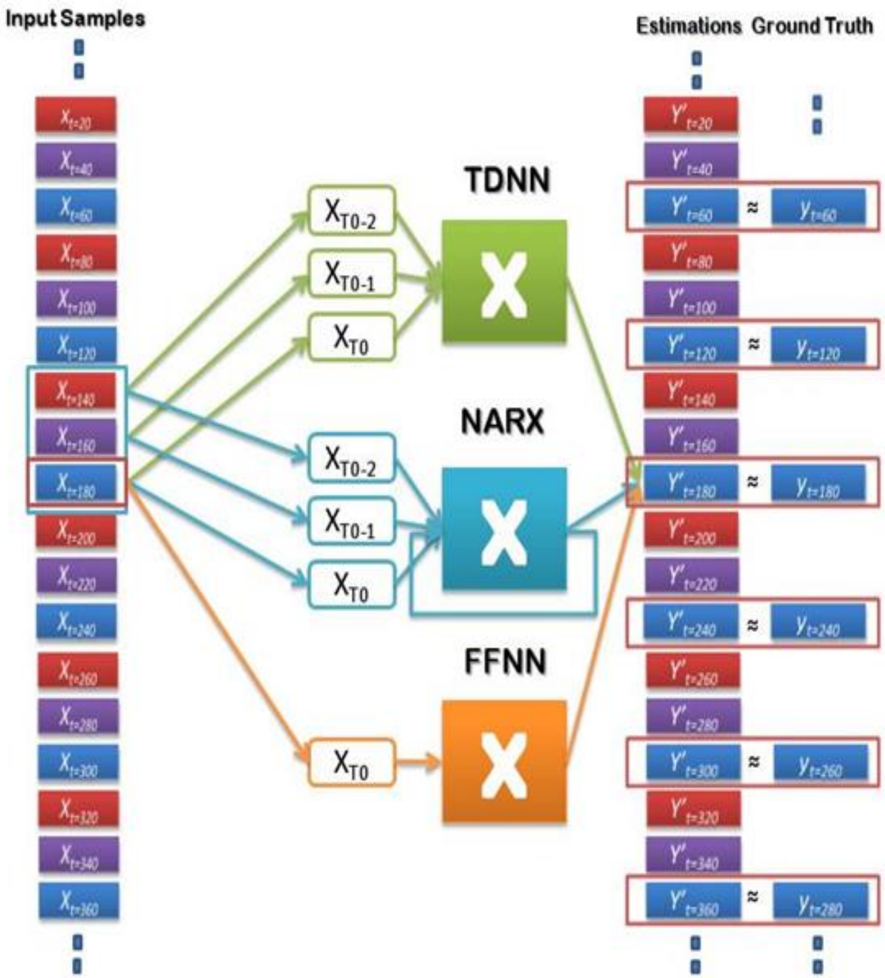


TDNN : a BPNN fed with current and pastsensor responses .
Hyperparameters: # of hidden neurons, length of tapped delay line.



NARX : a BPNN fed with current and past sensor responses + feedback of past estimations.
Hyperparameters: # of hidden neurons, length of tapped delay line.

Train & Test Procedure



GT @ 1sample/min
Sensor data @ 20 sec/min
10k Training samples (1° wk)
10k Validation samples (2° wk)
20k Test samples (3° & 4° wk)

Validation set used for:
-Hyperparameters optimization
-Uncertainty Estimation

Performance evaluation
-30x averaging procedure for initial weight choice dependance reduction

Obtaining Stochastic Estimations

By using validation set data we estimated the empirical predictive error (*err*) distribution, given target concentration estimation *y'*:

$$p(err|y' \in a_i)\ ,$$

…. We have fit it with a gaussian model (tested with KS-test) and used to compute

Mean μ_a^{err} and standard deviation σ_a^{err}

O

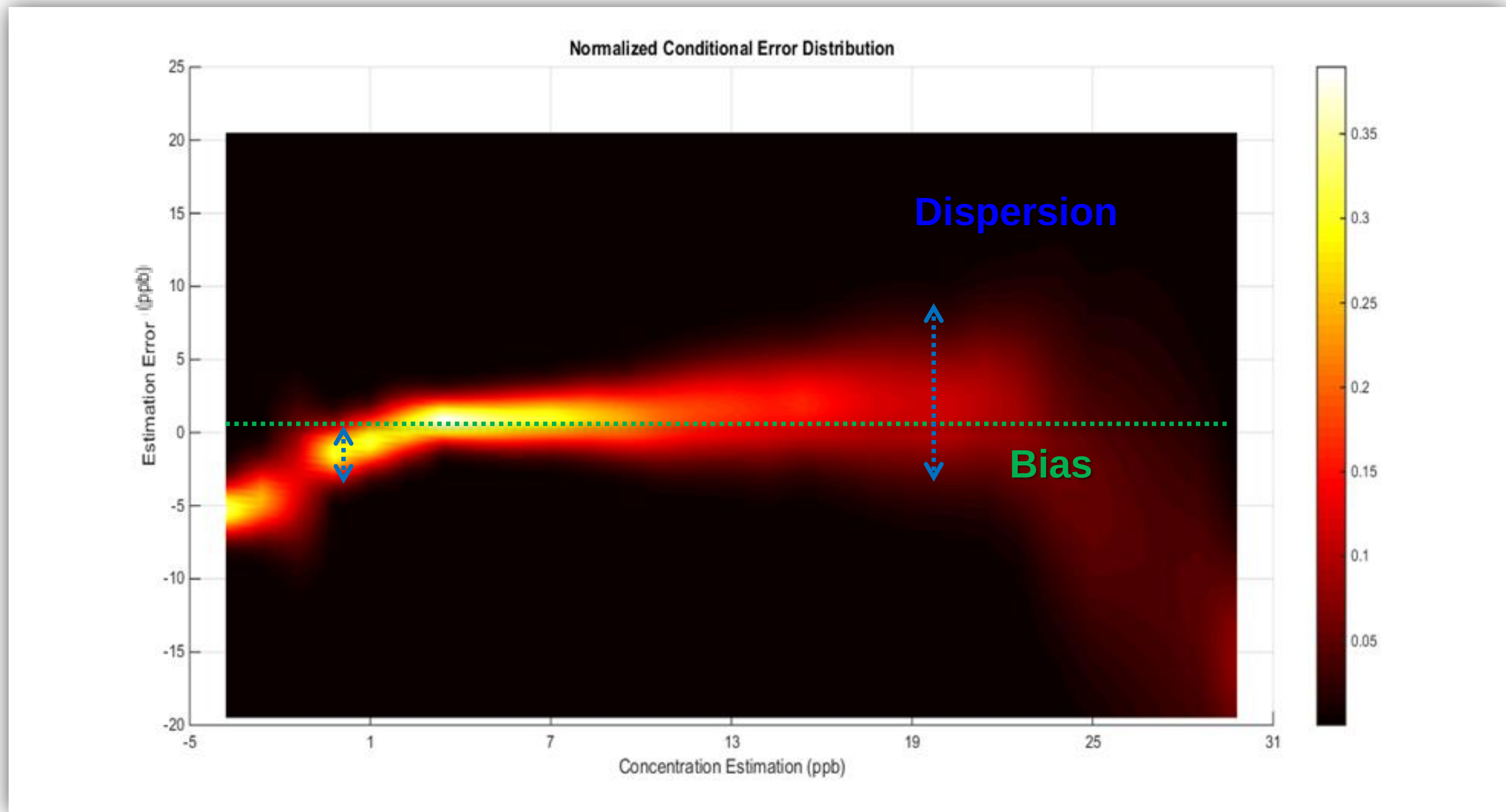
…. to obtain biased uncertainty bars for estimation performed at time *t*, using a coverage factor of 1σ:

$$\mu_{a,t}^{err} - c(\sigma_{a,t}^{err}) \leq (y'(\vec{x},t) - y(t)) \leq \mu_{a,t}^{err} + c(\sigma_{a,t}^{err}),$$

where $y'(\vec{x},t)$ is the network output,

Ref.: J. Monroy et al., Sens & Act. B, Chemical , 2013

Obtaining Stochastic Estimations



Note that dispersion of *p(err|y')* increase at higher y' values

Evaluation of uncertainty estimation

- We have chosen Negative Log Prediction Density loss as performance index for uncertainty estimation procedure:

$$NLPD = \frac{1}{2N}\left\{\sum_{t=1}^{N}\left[\log(var_t) + \frac{(y(t)-\mu_t)^2}{var_t}\right]\right\} + c$$

- Note that it both penalice over and under confident predictions

Results:

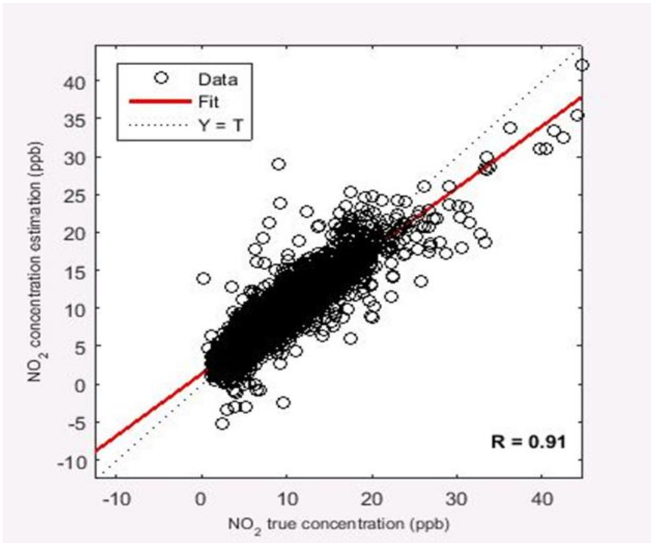
TABLE 1: RESULTS OF THE COMPARISON TESTS FOR ESTIMATION OF NO_2 CONCENTRATIONS (TEST SET VALUES).

Neural Net	Input (Sensors)	Hyper Parameters	MAE (ppb)	MRE	NLPD
FFNN	NO, NO_2, O3, Rh, T	HN=5	1.50(std=0.06)	0.25	2.15(std=0.03)
	NO, NO_2, O3	HN=5	1.58(std=0.04)	0.28	1.98(std=0.01)
TDNN	**NO, NO_2, O3, Rh, T**	**HN=5, ID=0:6**	**1.27(std=0.10)**	**0.22**	**1.78(std=0.05)**
	NO, NO_2, O3	HN=5, ID=0:6	1.33(std=0.05)	0.24	1.78(std=0.02)
NARXNN	NO, NO_2, O3, Rh, T	HN=5, ID=0:6, FD=1:5	1.30(std=0.15)	0.21	1.82(std=0.10)
	NO, NO_2, O3	HN=5, ID=0:6, FD=1:5	1.40(std=0.10)	0.24	1.87(std=0.21)

Table 1: Results obtained upon 30 different executions by the proposed architecture by the use of the complete chemical sensor array (+environmental variables). HD = Hidden Number, ID = Input Delay and FD = Feedback Delay.

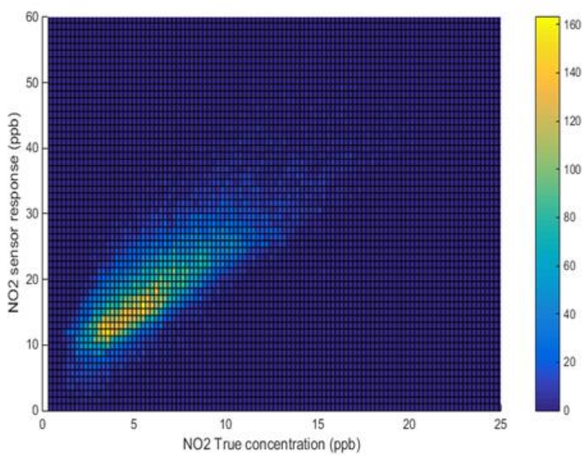
- **The TDNN overcome FFNN in every performance index measurement.**
- **Statistically significant advantage (*t-test*) are measured for DNNs over the static state of the art approach (>15% on MAE).**

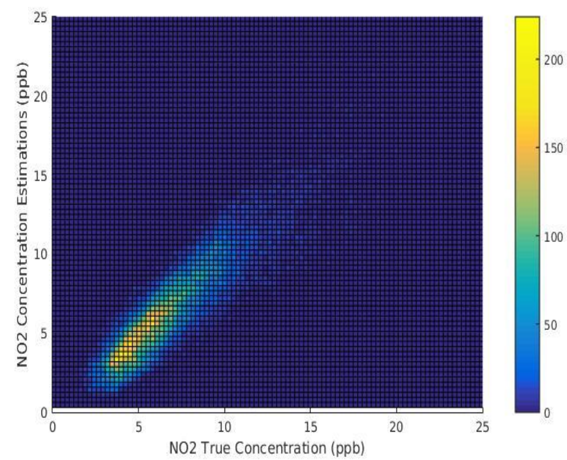
Results (Graphically):



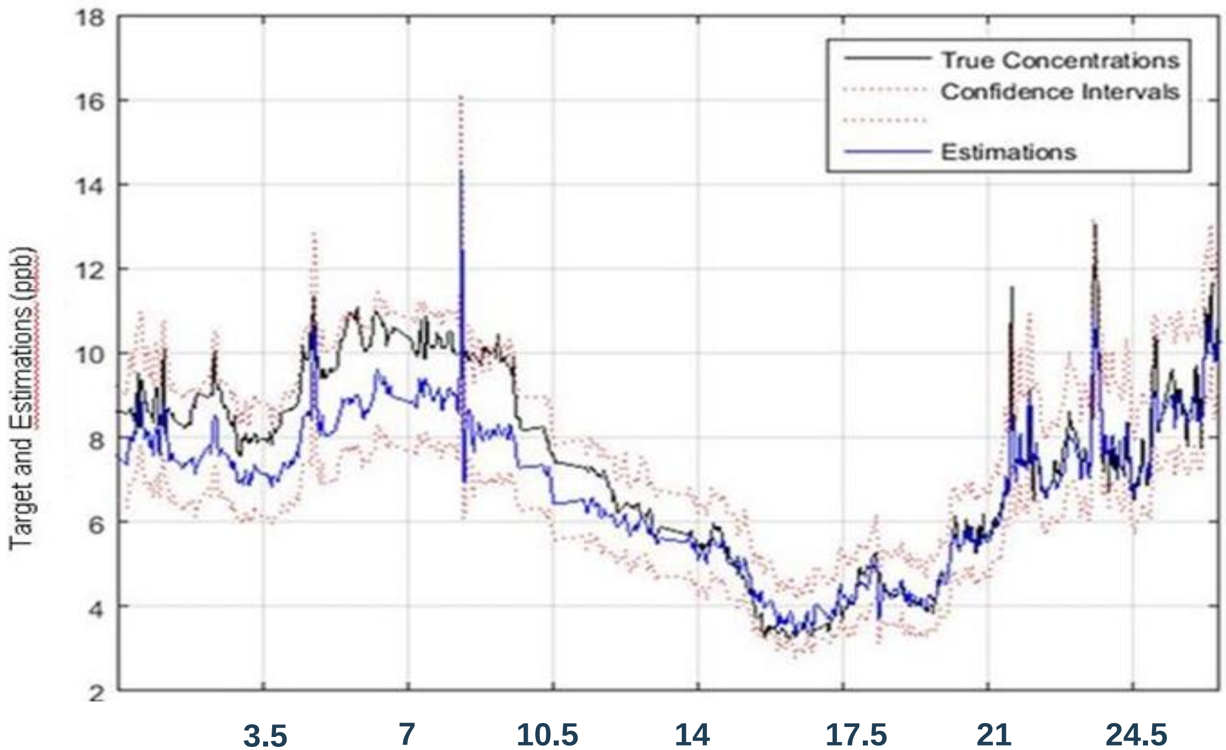
Correlation Factor is now exceeding 0.90

Of course, the correlation/distribution plot in the 3° and 4° week is significantly ameliorated



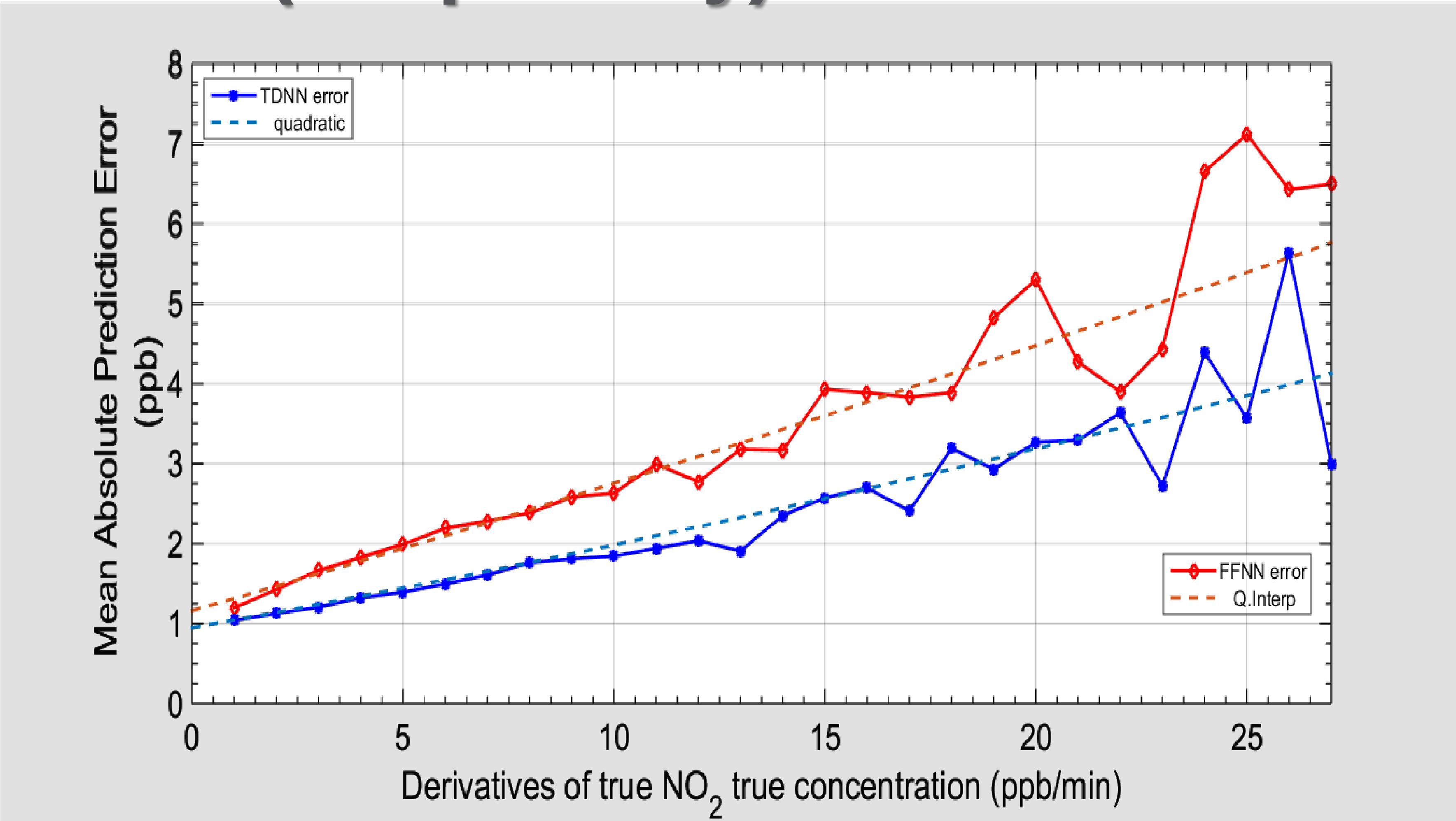


Results (Graphically):



We have now a stochastic prediction for NO_2 capable to follow rapid transients…

Results (Graphically):



… and reduce the error induced by rapid transients with respect to state of the art approach.

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Ref.: S. De Vito et al., Accepted Sens & Act. B, Chemical 2016

Further Results (other species):

TABLE 2: COMPARISON OF DIFFERENT CALIBRATION METHODOLOGIES FOR ESTIMATION OF NO_2, O_3, NO_x CONCENTRATIONS OVER TEST SET.

Target	Calibration Methodology	MAE (ppb)	STDERR (ppb)	CC	MRE (perc)
NO_2	Static Univariate	1.68	1.75	0.80	31%
NO_2	Static Multivariate	1.50	1.69	0.84	25%
NO_2	**Dynamic Multivariate (TDNN)**	**1.27**	**1.32**	**0.91**	**22%**
O_3	Static Univariate	8.30	6.87	0.50	90%
O_3	Static Multivariate	7.90	5.21	0.82	70%
O_3	**Dynamic Multivariate (TDNN)**	**7.45**	**5.10**	**0.83**	**42%**
NO_x	Static Univariate	2.14	2.65	0.82	31%
NO_x	Static Multivariate	1.95	2.39	0.85	29%
NO_x	**Dynamic Multivariate (TDNN)**	**1.37**	**1.61**	**0.94**	**20%**

Table 2: Comparison of the results obtained, respectively, with Univariate, Multivariate and Dynamic Multivariate Calibration (TDNN).

Conclusions

- We have observed and shown degradation of prediction capabilities of calibrated microsensors based AQ monitors in presence of rapid changes in pollutants real concentrations.

- We have proposed a new Dynamic ML based stochastic approach to calibration.

- Tests on multiple weeks real world deployments confirm that the dynamic approaches outperform significantly the state of the art one for multiple pollutants.

Thank You for Your Attention!

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