



Data Assimilation and Machine Learning Science at ECMWF

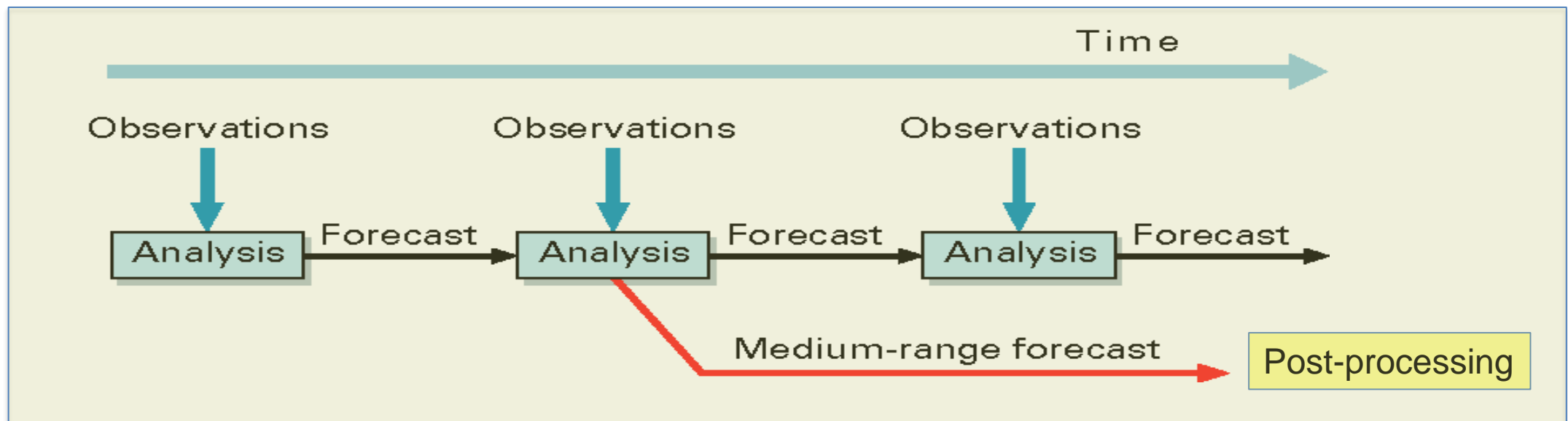
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1: ECMWF

2: École des ponts ParisTech



All components of the NWP workflow can potentially be improved by ML technologies:

- a) **Observations:** Quality Control decisions, Bias correction, Observation operator
- b) **Forecast:** Model error correction, Model identification, model development
- c) **Analysis:** Model error estimation and correction, Model parameter estimation, linearised/adjoint models for Var
- d) **Post-processing:** Ensemble/Determ. post-processing, Sig. Weather ident.,

Data Assimilation and Machine Learning

- There is (almost) universal agreement that ML can be useful in NWP and Climate Prediction
- Maybe something that is not so uncontentious is the following:

*“From a methodological point of view, ML **is not a conceptual jump** from the current Data Assimilation theoretical framework: in fact, it is a particularisation of DA methodology”*

- We already do ML in operational Data Assimilation: It is called weak-constraint 4D-Var!

Data Assimilation and Machine Learning

Weak Constraint 4D-Var Loss Function



Generic ML/DL Loss Function

$$J_{WC4DVar}(\mathbf{x}_0, \boldsymbol{\eta}) = J_B + J_O + J_Q =$$

$$\frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_0^b)$$

$$+ \frac{1}{2} \sum_{i=0}^N (\mathbf{H}_i(\mathbf{x}_i) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (\mathbf{H}_i(\mathbf{x}_i) - \mathbf{y}_i)$$

$$+ \frac{1}{2} \sum_{i=1}^N \left(\mathbf{x}_i - \mathbf{M}_i(\mathbf{x}_{i-1}, \boldsymbol{\eta}) \right)^T \mathbf{Q}_i^{-1} \left(\mathbf{x}_i - \mathbf{M}_i(\mathbf{x}_{i-1}, \boldsymbol{\eta}) \right)$$

~~$$J_{ML}(\mathbf{x}_0, \boldsymbol{\eta}) =$$~~

~~$$\frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_0^b)$$~~

~~$$+ \frac{1}{2} \sum_{i=0}^N (\mathbf{H}_i(\mathbf{x}_i) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (\mathbf{H}_i(\mathbf{x}_i) - \mathbf{y}_i)$$~~

~~$$+ \frac{1}{2} \sum_{i=1}^N \left(\mathbf{x}_i - \mathbf{M}_i(\mathbf{x}_{i-1}, \boldsymbol{\eta}) \right)^T \mathbf{Q}_i^{-1} \left(\mathbf{x}_i - \mathbf{M}_i(\mathbf{x}_{i-1}, \boldsymbol{\eta}) \right)$$~~

Notes: (Brajjard et al., 2020; Bocquet et al., 2020; Farchi et al., 2020)

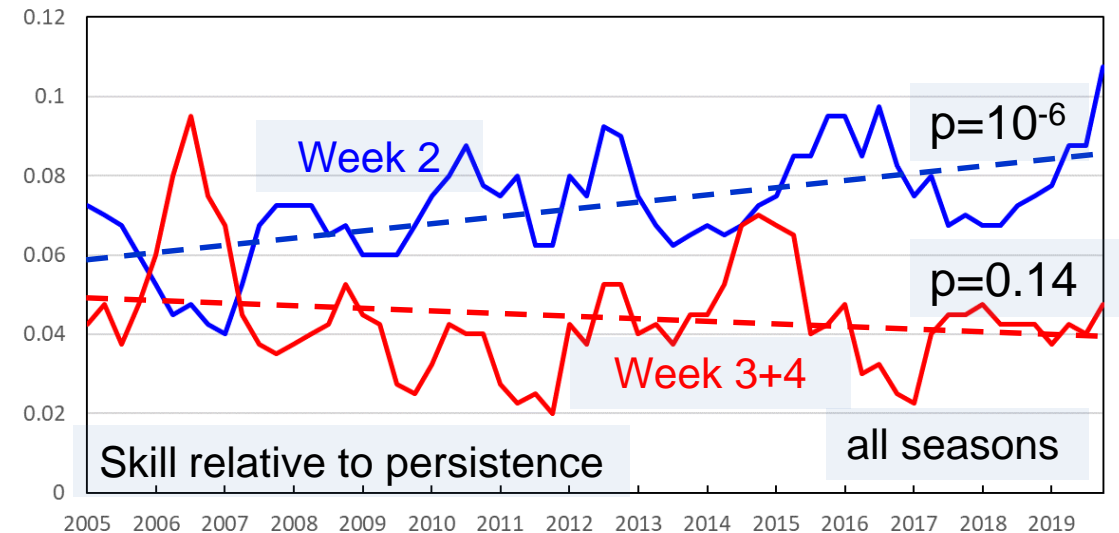
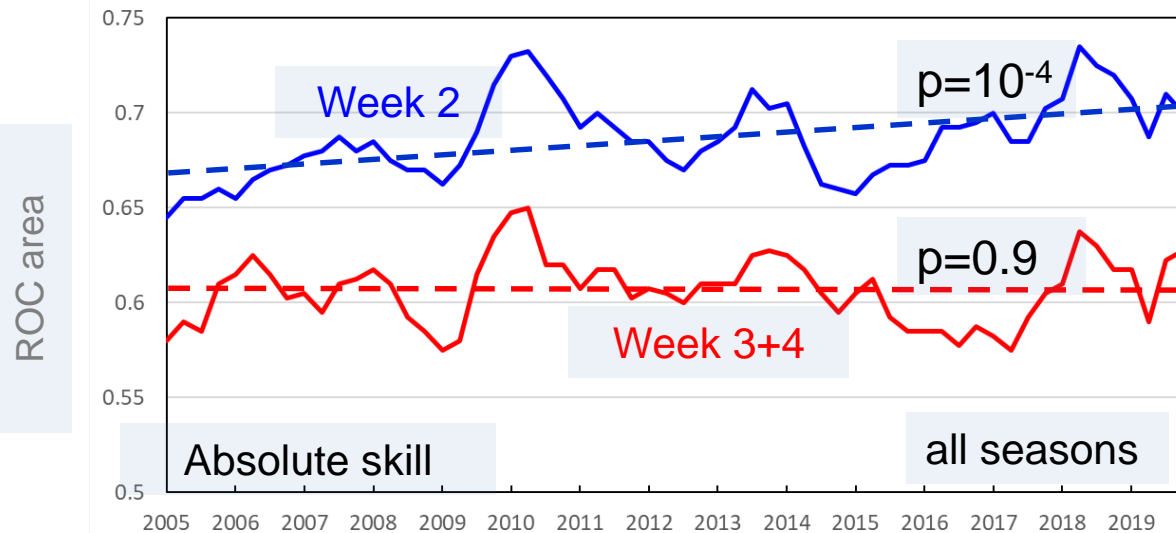
1. ML/DL models are not used for state estimation $\rightarrow J_B = 0$
2. ML/DL loss functions typically assume full, noiseless observations ($\mathbf{H}_i = \mathbf{I}, \mathbf{R}_i \rightarrow 0$) $\rightarrow J_O = 0$
3. ML/DL models can optionally have a regularization term function of the ANN model parameters $\mathcal{L}(\boldsymbol{\eta}) = \mathcal{L}(\mathbf{W}, \mathbf{b})$, e.g. Tikhonov regularisation, drop-out, etc.

Data Assimilation and Machine Learning

- Given that ML/DL can be seen as a particularisation of standard Data Assimilation methodology, is the current excitement about it justified?
- We believe the answer is yes, for at least two reasons:
 1. Technically the explosion of ML/DL has provided a wealth of efficient, easy to use open source software that can be easily repurposed for one's applications: "the democratisation of Machine Learning"
 2. In the Earth Sciences, it has brought into prominence the idea that the current and ever-increasing wealth of **geophysical observations can be directly used to improve/extend/correct our forecast models**

Data Assimilation and Machine Learning

- Improving forecast models can be considered the most urgent requirement to advance predictive skill, especially on extended, sub-seasonal and seasonal time scales
- Traditionally, DA algorithms have used a perfect model assumption and aimed at reducing random initial conditions errors: this brings steady progress up to ~2 weeks, but not much is visible beyond two weeks
- Can we deploy ML to break the 2-week Lorenz predictability barrier?

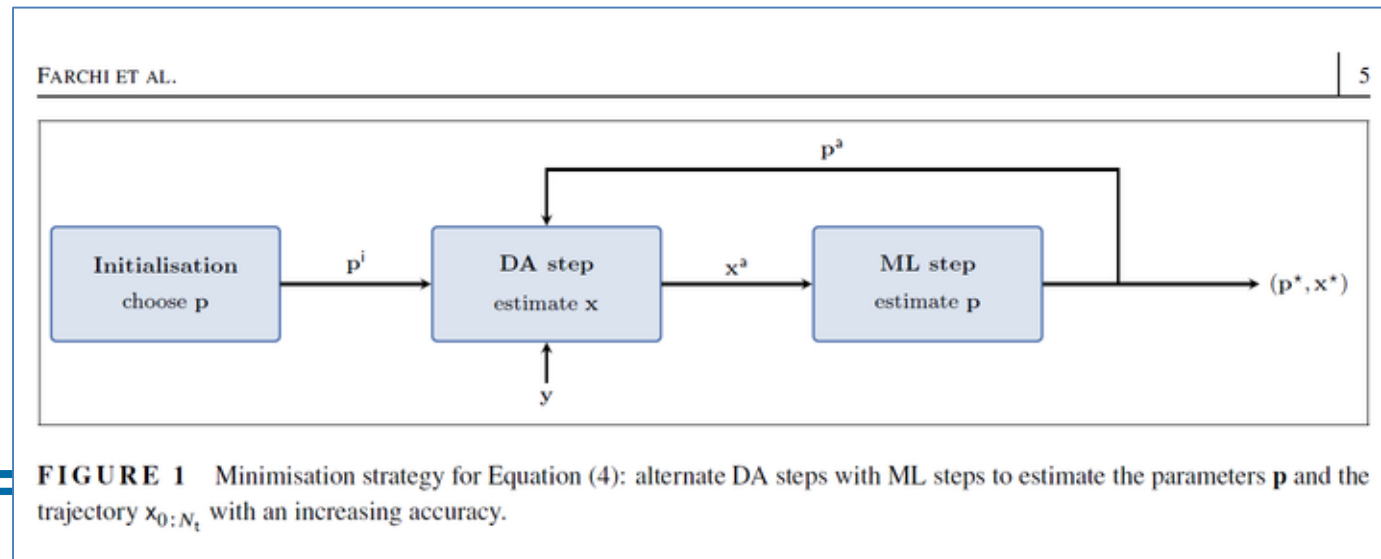


Data Assimilation and Machine Learning

- Ideally we would like to estimate the state and the model consistently and simultaneously, i.e. to solve the **full Bayesian estimation problem** (Bocquet et al., 2020):

$$p(\mathbf{x}_{0:K}, \mathbf{A} | \mathbf{y}_{0:K}) = \frac{p(\mathbf{y}_{0:K} | \mathbf{A}, \mathbf{x}_{0:K}) p(\mathbf{x}_{0:K} | \mathbf{A}) p(\mathbf{A})}{p(\mathbf{y}_{0:K})}$$

- In low-order geophysical systems it has been shown to be possible to solve this problem of state and model estimation (e.g. Brajard et al., 2020, Bocquet et al., 2020, Bocquet et al., 2019) using a coordinate descent approach:



Data Assimilation and Machine Learning

- How can we adapt this general recipe to operational NWP and Climate prediction? There are two issues:
 1. We do not have enough time to iterate the DA and ML steps in real time NWP;
 2. We have a much more complex model to deal with ☹, but we do not start from zero, but from a very good model 😊!
- These two features of the NWP/Climate prediction endeavour point to two ways of attacking the combined state-model estimation problem in 4DVar:
 1. **Model Parameter estimation**
 2. **Model Error estimation and correction**

Combining DA and ML: Model Parameter Estimation

- In Model Parameter estimation we start from a fundamental assumption:
“the model is structurally sound, model errors (mainly) arise from incorrect settings of its parameters (or parameters of their pdfs, in a stochastic model framework)”.
- This assumption has the big advantage that it drastically reduces the hypothesis space of our ML model to that of the model parameters ($\sim O(10^2)$)
- Traditionally, these parameters are hand-tuned comparing short and long forecasts (and ensemble of forecasts) to observations/analyses. This is computationally expensive and labour intensive.
- Assuming the model parameters have a strong correlation with the observed variables (Identifiability condition: Navon, 1997), we can add them to the control vector of the analysis (**Augmented Control Vector**, see Ruiz et al., 2013, for a review), both in Ensemble and Variational DA

Combining DA and ML: Model Parameter Estimation

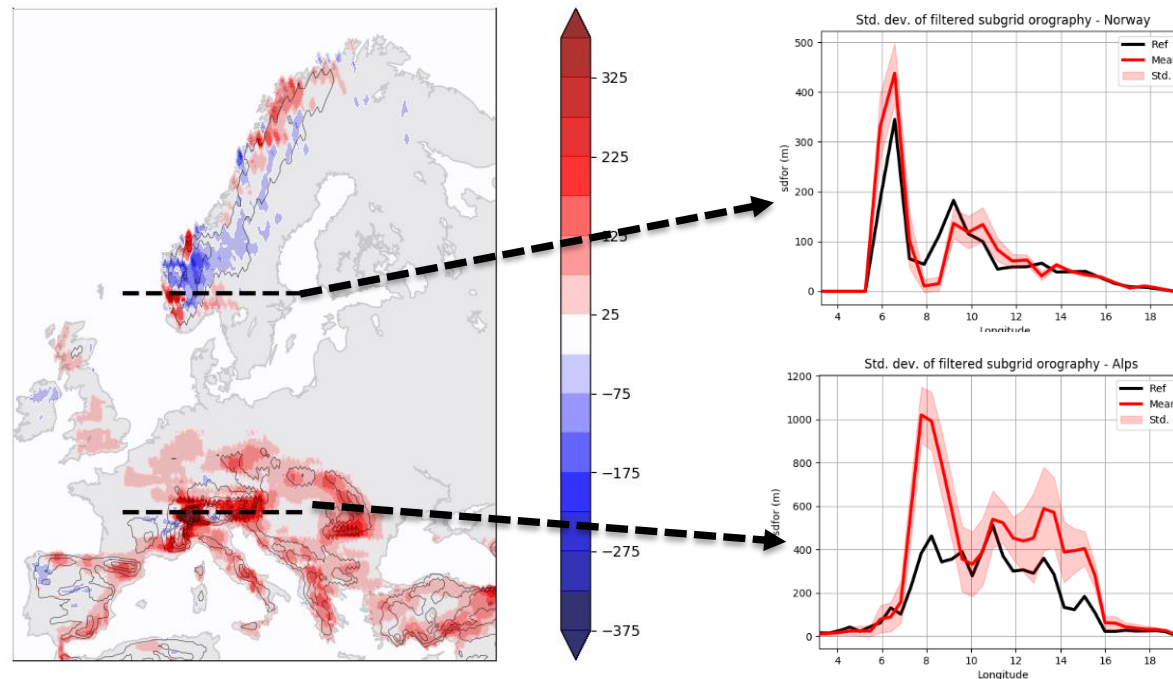
- Augmented Control Vector in 4DVar:

$$J_{4DVar}(\mathbf{x}_0, \mathbf{p}) = J_B + J_P + J_O = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}(\mathbf{p} - \mathbf{p}^b)^T \mathbf{B}_p^{-1}(\mathbf{p} - \mathbf{p}^b) + \frac{1}{2} \sum_{i=0}^N (H_i \circ M_i(\mathbf{x}_0; \mathbf{p}) - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (H_i \circ M_i(\mathbf{x}_0; \mathbf{p}) - \mathbf{y}_i)$$

- \mathbf{p} is the set of model parameters (or fields of those) that are estimated together with the state. (This could also be applied to uncertain parameters of the forward model H)
- This approach has been around in atmospheric data assimilation since at least the mid '90s, but results have been rather inconsistent in realistic applications
- With the current and projected wealth of available observations (ECMWF DA ingests ~40 million obs every 12h!) time is ripe for revisiting this idea

Combining DA and ML: Model Parameter Estimation

Example: Online Estimation of the “standard deviation of subgrid orography” in the IFS Orographic Drag scheme (S. Massart, ECMWF)



- Identifiability: Surface pressure is sensitive to orography, 4DVar can constrain the parameter through surf. press. observations
- Preliminary results show improved surface pressure forecast skill!

Analysis increments of estimated StDev orography (left)
Cross section of default (black) and estimated (red, mean + spread) parameter values (right)

Combining DA and ML: Model Error Estimation and Correction

- In Model Parameter estimation we have made the assumption that a perfect model is a model with optimal parameter values;
- However models (model parameterisations) have also non-negligible **structural uncertainties** (e.g., BL turbulence, cloud convection), which cannot be resolved by tuning of the closure parameters;
- A different approach is to abandon the perfect model assumption and consider the evolution of the state given by the knowledge-based model plus a **residual model** error component:

$$\mathbf{x}_k = M_k(\mathbf{x}_{k-1}) + \boldsymbol{\eta}_k(\mathbf{x}_{k-1}) = M_k(\mathbf{x}_{k-1}) + M_k^{ML}(\mathbf{x}_{k-1})$$

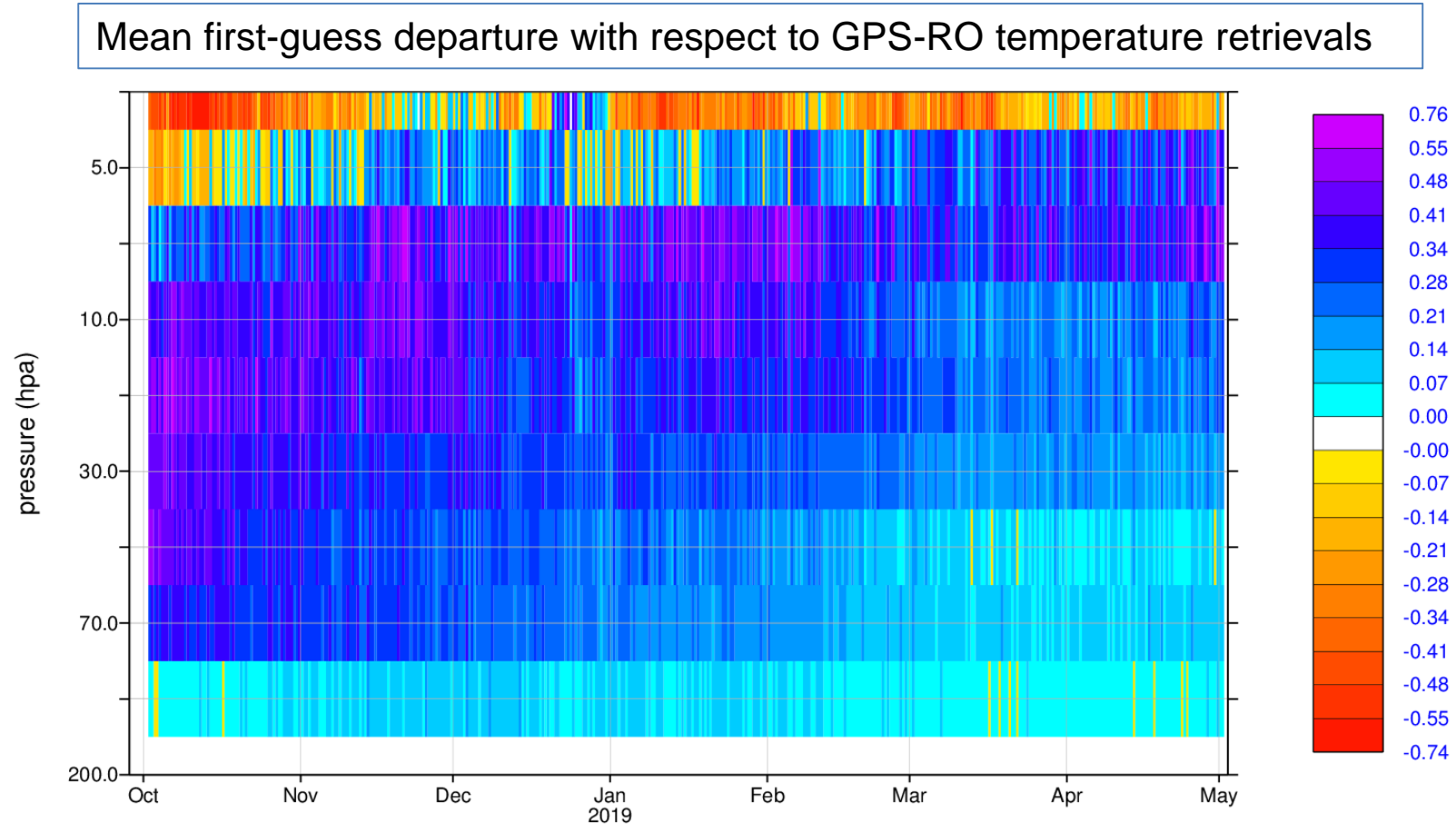
- In Data Assimilation this idea is called **weak constraint 4DVar** (Sasaki, 1970)

Weak Constraint 4D-Var

- The ECMWF version of WC-4DVar works by estimating (“learning”) a constant model error tendency over the assimilation window (12 hours)
- The background (and first guess) model error is the previous window’s estimate (we do not have a predictive model of model error!)
- This means that our model error formulation targets errors which are slowly evolving on the timescale of the assimilation window (ie, 12 hours) and large scale with respect to typical background errors
- These insights are the basis of the success of the latest WC-4DVar implementation in dealing with **stratospheric model biases** (Laloyaux et al., 2020a, b)

Weak Constraint 4D-Var

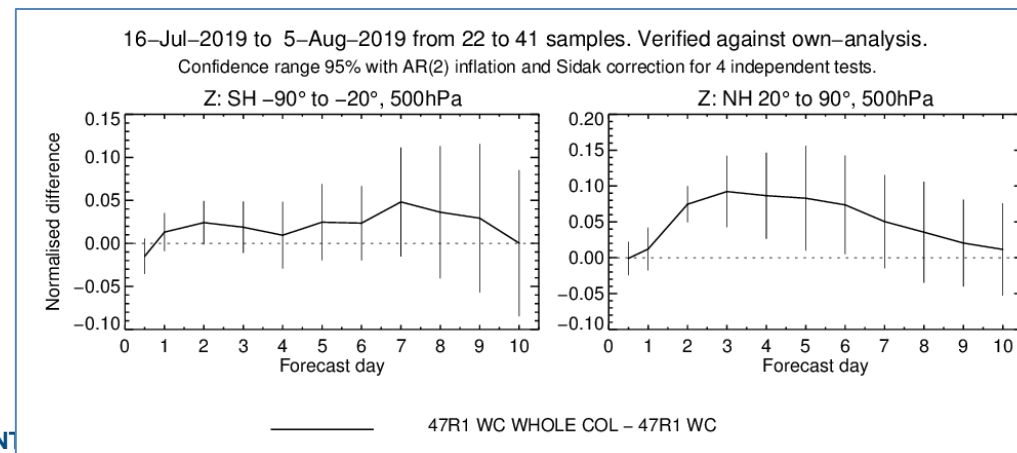
- WC-4DVar gradually learns a model error tendency correction and applies it during the assimilation cycle
- WC-4DVar is **an online machine learning** algorithm for model error estimation and correction



From Laloyaux et al, 2020b

Weak Constraint 4D-Var

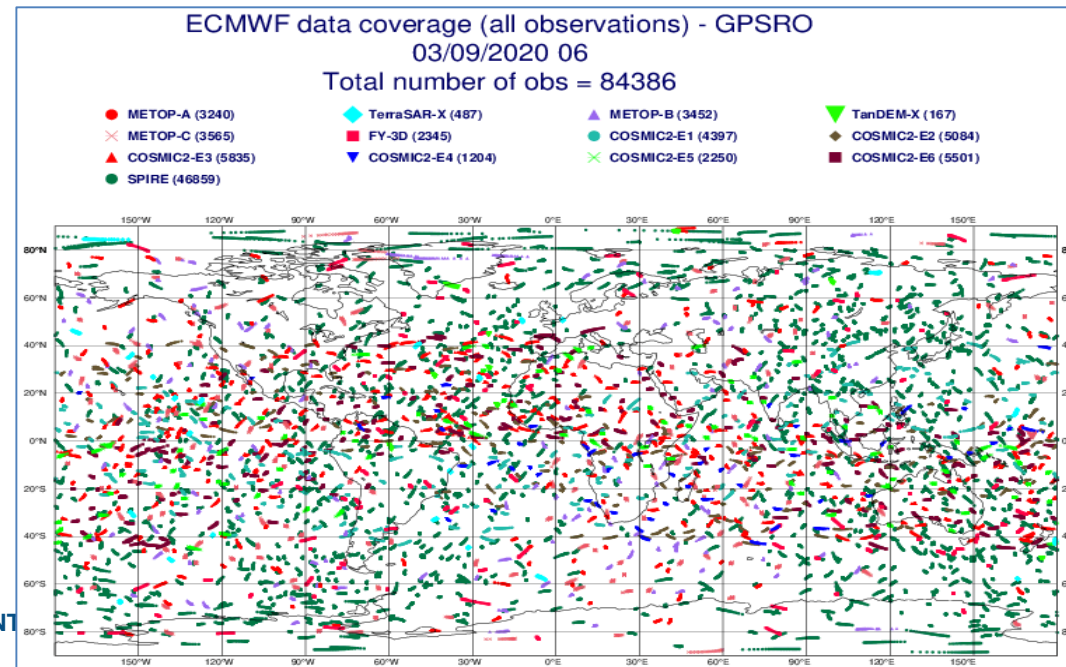
- Current version of WC-4DVar is a step change wrto previous versions, but it is not the end of the story (so far):
 - WC-4DVar reduces stratospheric fcst temperature bias ~ completely against BC corrected obs (radiances), by 30-40% against non-bias corrected obs (Radiosondes, GPS-RO)
 - Current WC-4DVar has little impact on wind systematic errors
 - Current WC-4DVar is only active above ~100hPa. Letting it loose on full atmospheric column leads to unacceptable forecast skill degradation in troposphere



Combining DA and ML: Model Error Estimation and Correction

What can Machine Learning bring to the problem of model error identification and correction?

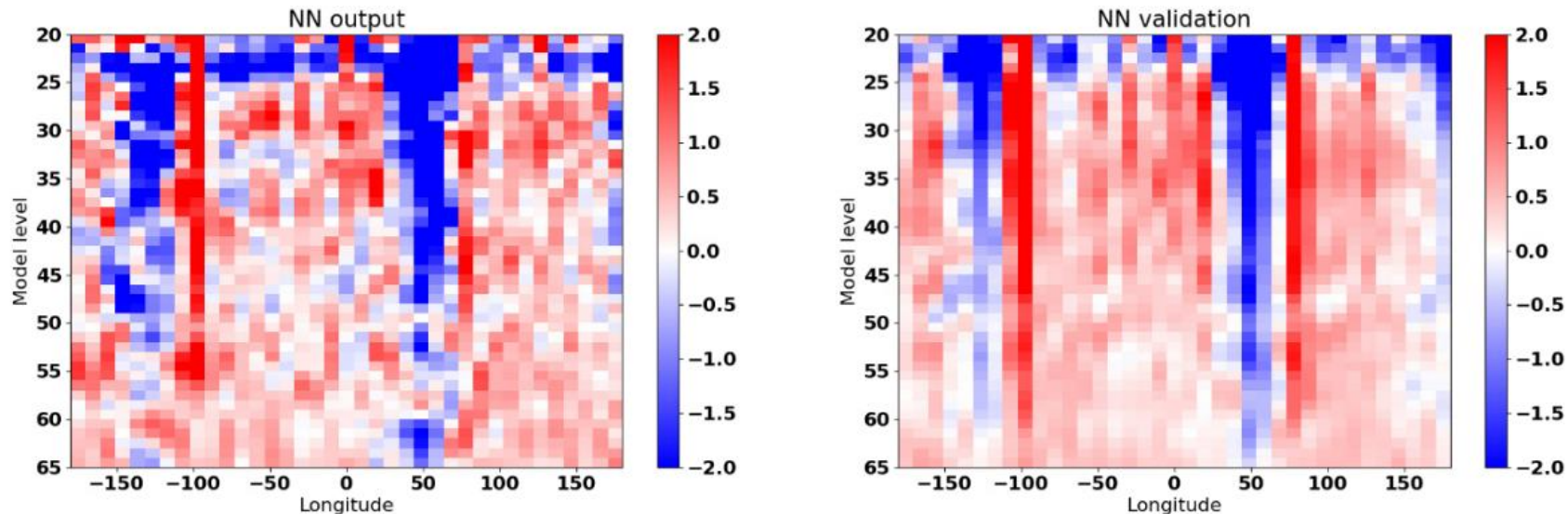
- Basic idea: Train an Artificial Neural Network to “learn” the statistically predictable part of model error
- The training of the Neural Network can be realised in at least two ways
- The most direct way is to train the ANN on a database of observation-background (O-B) departures, choosing an approx. homogeneous, dense and unbiased observing system, eg GPS-RO:



Combining DA and ML: Model Error Estimation and Correction

- The idea of training the ML model from observation departures has the advantage of bypassing the assimilation cycle, which avoids the systematic errors present in the analyses
- However it introduces other complications, e.g. lack of homogeneous coverage, need of long timeseries, how to extrapolate the corrections to unobserved locations and unobserved state variables (ie, how to make an ANN produce an analysis?)

O-B on 1-5-2019 averaged between 10S and 20N (left) and the prediction of the Convolutional Neural Network (right)



Combining DA and ML: Model Error Estimation and Correction

- The other possibility is to train the ML model on a database (fixed or rolling) of **analysis increments**, again under the assumption that the learnable part of the increments is due to systematic model deficiencies
- This idea is not new in Data Assimilation, e.g. Dee, 2005, proposed an online version of this idea:

“In the presence of bias, therefore, certain components of the increments are systematic and therefore predictable. ... Provided the predictable part of the increment can be attributed to model errors, the algorithm

$$\mathbf{dx}_k^p = \mathbf{f}_k(\mathbf{dx}_{k-L}, \dots, \mathbf{dx}_{k-1}) \quad (43)$$

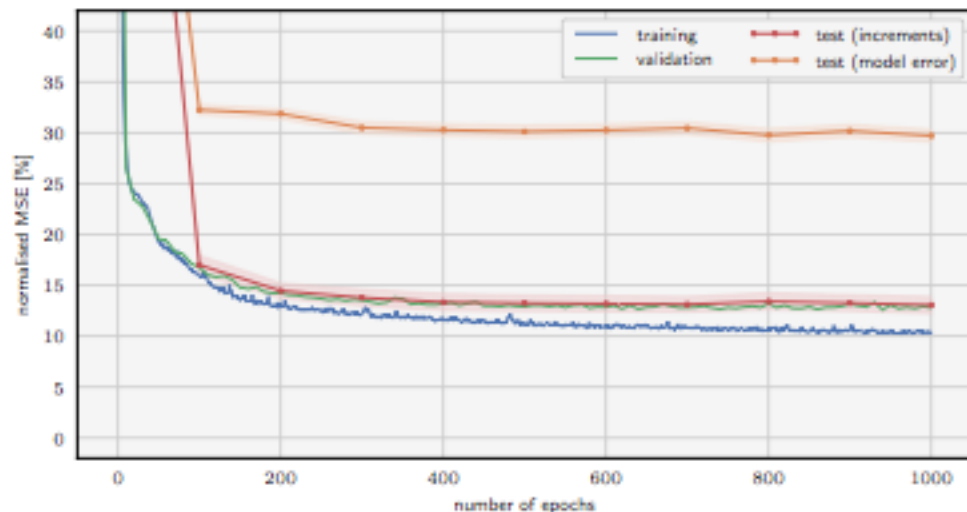
$$\mathbf{dx}_k = \mathbf{K}_k \left(\mathbf{y}_k - \mathbf{h}(\mathbf{x}_k^b - \mathbf{dx}_k^p) \right) \quad (44)$$

will correct the model background and produce unbiased analyses.”

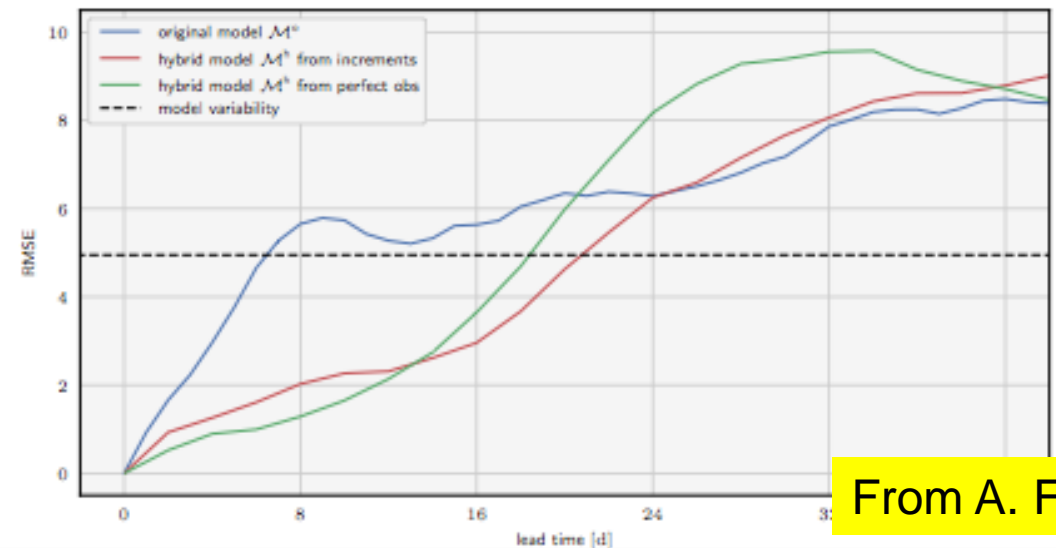
Combining DA and ML: Model Error Estimation and Correction

- We have tested this approach in a low order 2-level, 1600 variables QG model (Farchi et al., 2020; visit [poster space of Alban Farchi](#) for more details)
- The trained ANN can explain ~70% of the model error variance and when used in forecast mode to correct model errors can **~double the predictability horizon** of the forecasts!
- When the trained ANN is used in the DA cycle only, it **reduces RMS analysis errors by ~25%**
- How do these surprising results translate into operational-grade assimilation and modelling systems?

Training and test curves for the ANN



Evolution of the fcst RMSE



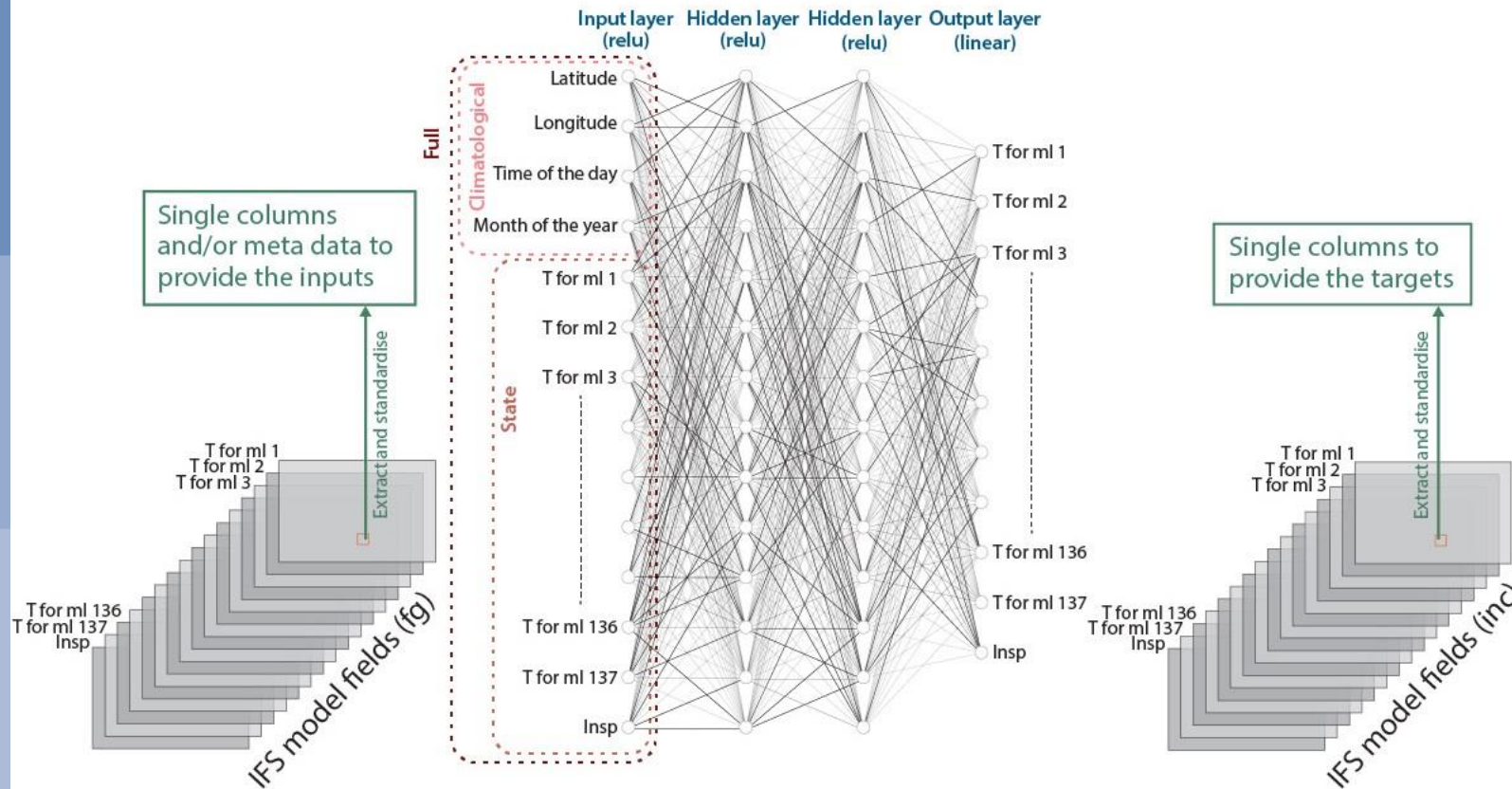
ORECAST

From A. Farchi

Combining DA and ML: Model Error Estimation and Correction

- We are testing this approach in the **operational version of the ECMWF IFS**, initial results are available in Bonavita and Laloyaux, 2020
- The size of the state vector is $\mathcal{O}(10^{10})$. Even assuming a much lower effective dimension for the model error vector, a primary design consideration for the ANN has been to reduce its size
- This led us to define a set of predictors made up of the concatenation of **climatological predictors** (time of day, month, lat, lon) and the **vertical columns** (137 levels) of the main prognostic variables of the model (t, l_{insp}, v_o, div, q).
- This choice to split **the 3D regression problem into a 1D x 2D problem** is similar to having a separable representation of a 3D covariance matrix and can be justified by two considerations:
 1. *We can consider the atmospheric flow to be subject to homogeneous dynamics and heterogeneous forcings;*
 2. *Physical parameterisations are computed and applied over model columns.*

Combining DA and ML: Model Error Estimation and Correction

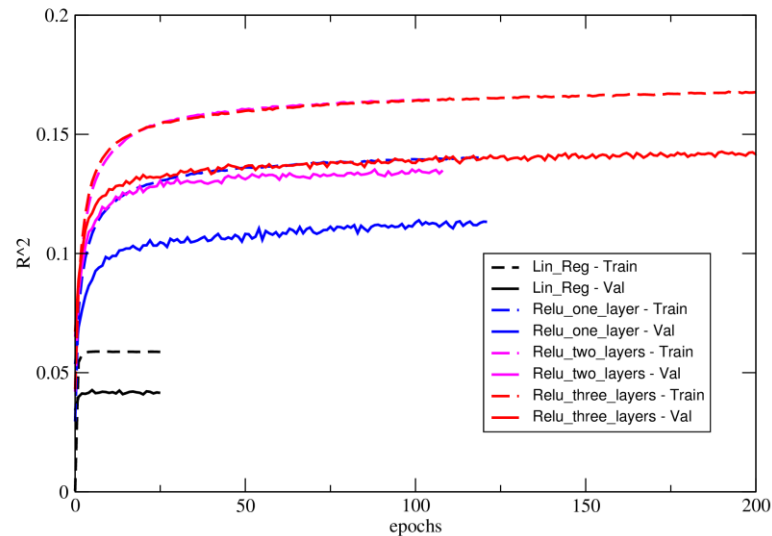


- Dense Neural Network with Relu activation
- **Three layers** with nonlinear activations give best results: problem with **only moderate nonlinearities**
- Dropout layers used to control overfitting, input/outputs pre-normalised for training, Adam minimiser
- Number of trainable parameters $\sim 6 \cdot 10^4$, size of training dataset $\sim 10^6$

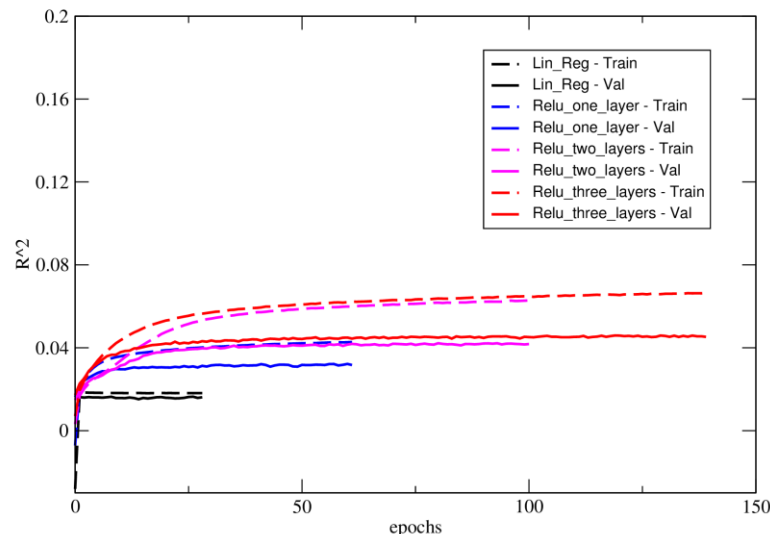
From Bonavita & Laloyaux, 2020

Combining DA and ML: Model Error Estimation and Correction

T_LNSP - Full Regressors



Vo_D - Full Regressors



- Training/Testing curves are shown in terms of explained variance (R^2)
- Saturation of explained variance is used as stopping criterion in the training
- **Mass (T, Insp) errors** can be better predicted (~14-15% explained variance) than **wind** (~4-5% explained variance) and **humidity** (~0%) errors.
- **State-dependent predictors (first guess values) have more predictive power than climatological predictors:** in forecast mode it is important to have an online model error correction.



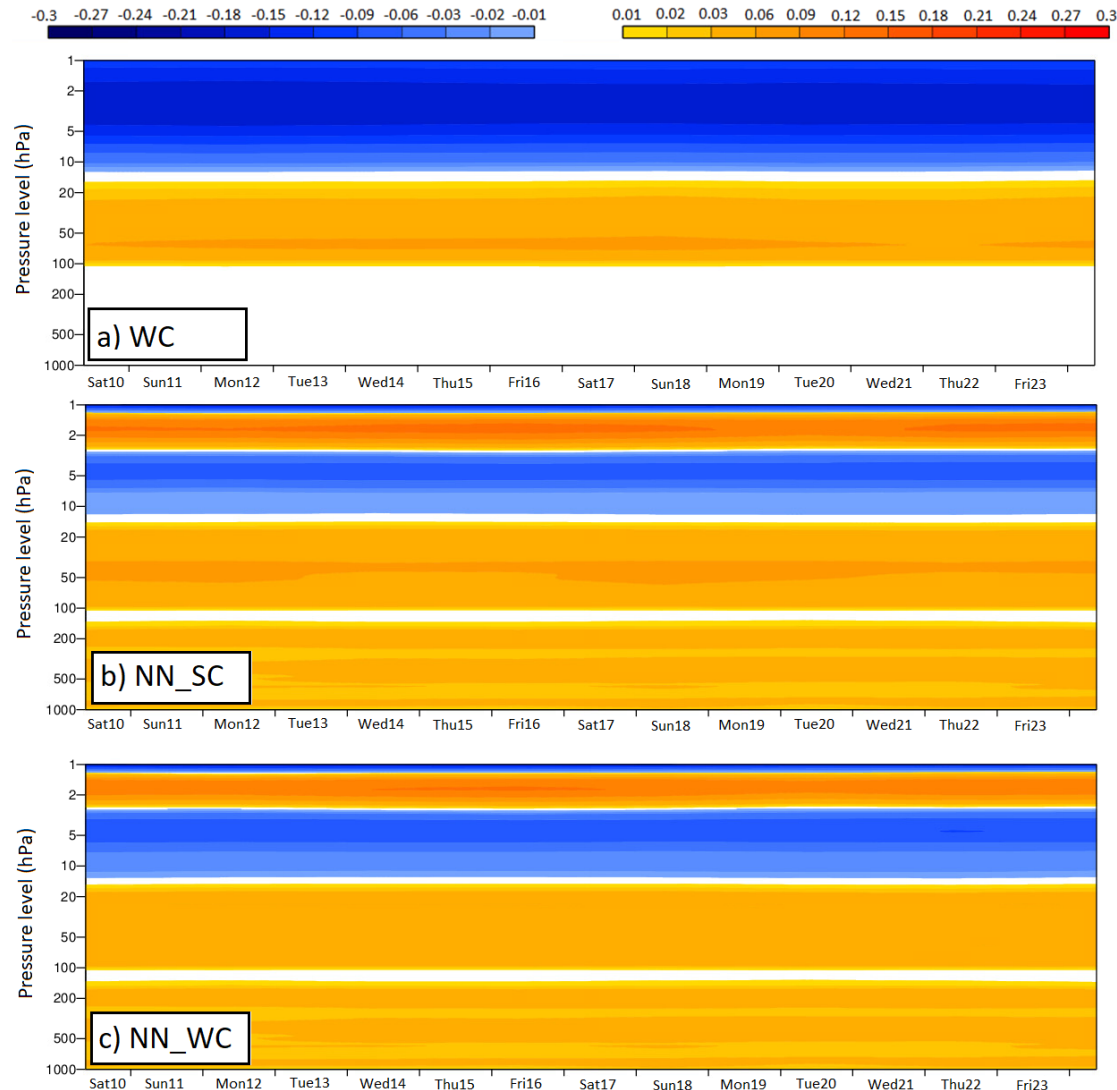
From Bonavita & Laloyaux, 2020

Combining DA and ML: Model Error Estimation and Correction

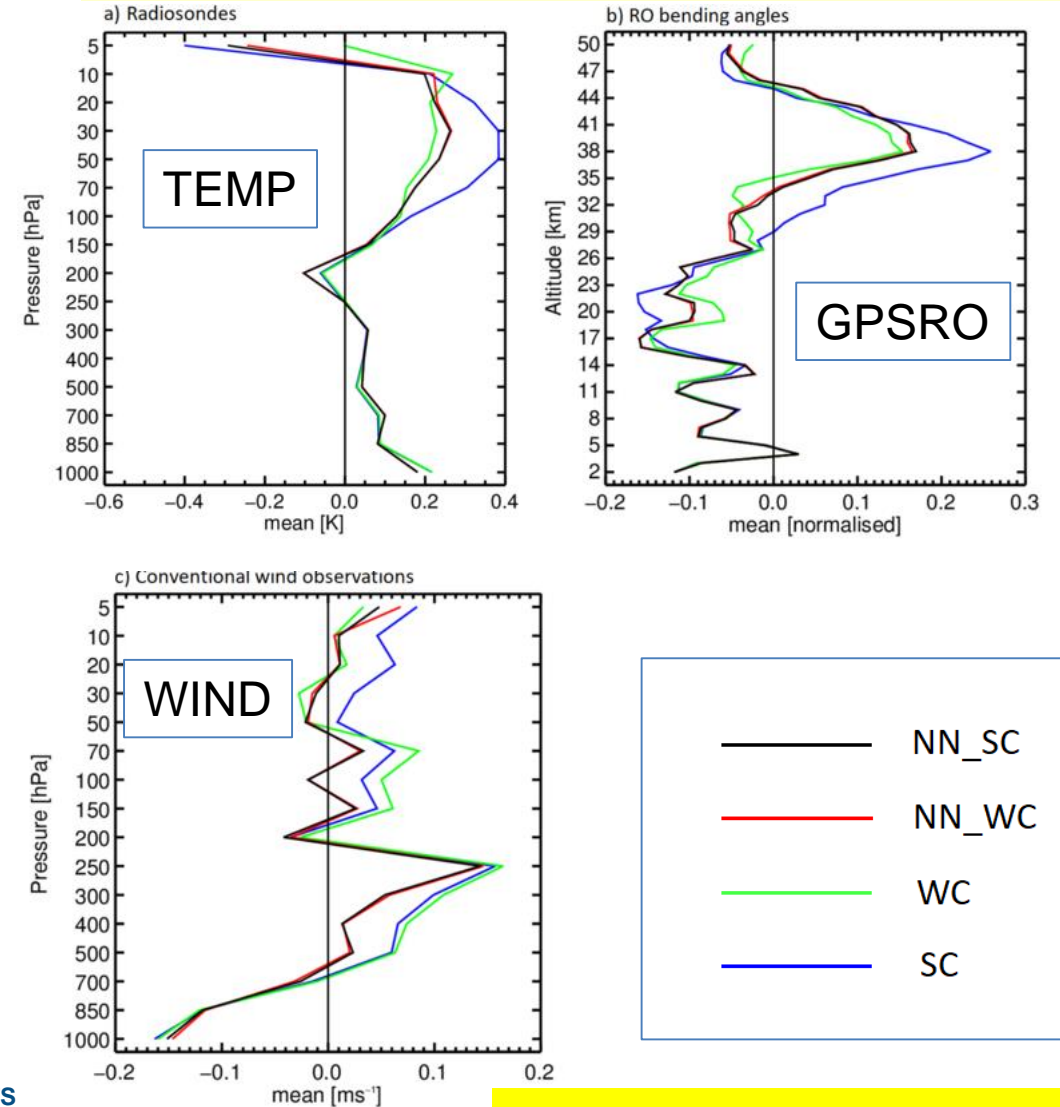
- So what happens when we use this trained Neural Network to correct model errors inside the data assimilation system of the operational IFS?
- The initial investigations focussed on two different configurations:
 - a) Use the NN model errors **instead of** the Weak Constraint 4D-Var model errors (**NN_SC** in the following);
 - b) Use the NN model errors as a **first-guess** for the Weak Constraint 4DVar (**NN_WC**)
- Baseline configuration was the currently operational version of Weak Constraint 4D-Var at full resolution (T1279, ~9km grid spacing) (**WC**) and the previously operational Strong Constraint 4D-Var (**SC**)

Model Error Estimation and Correction in the IFS: Mean errors

Globally-averaged Mean Temperature Correction



Globally-averaged Obs-Fg Mean Difference



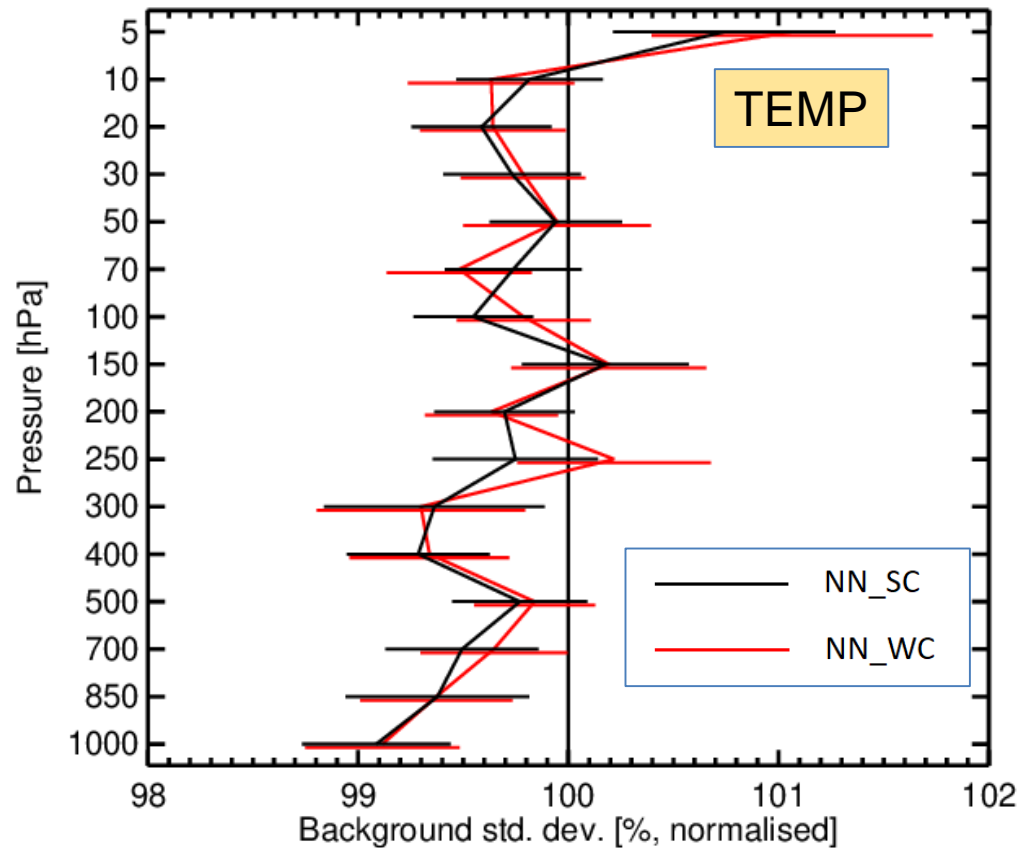
IRECASTS

From Bonavita & Laloyaux, 2020

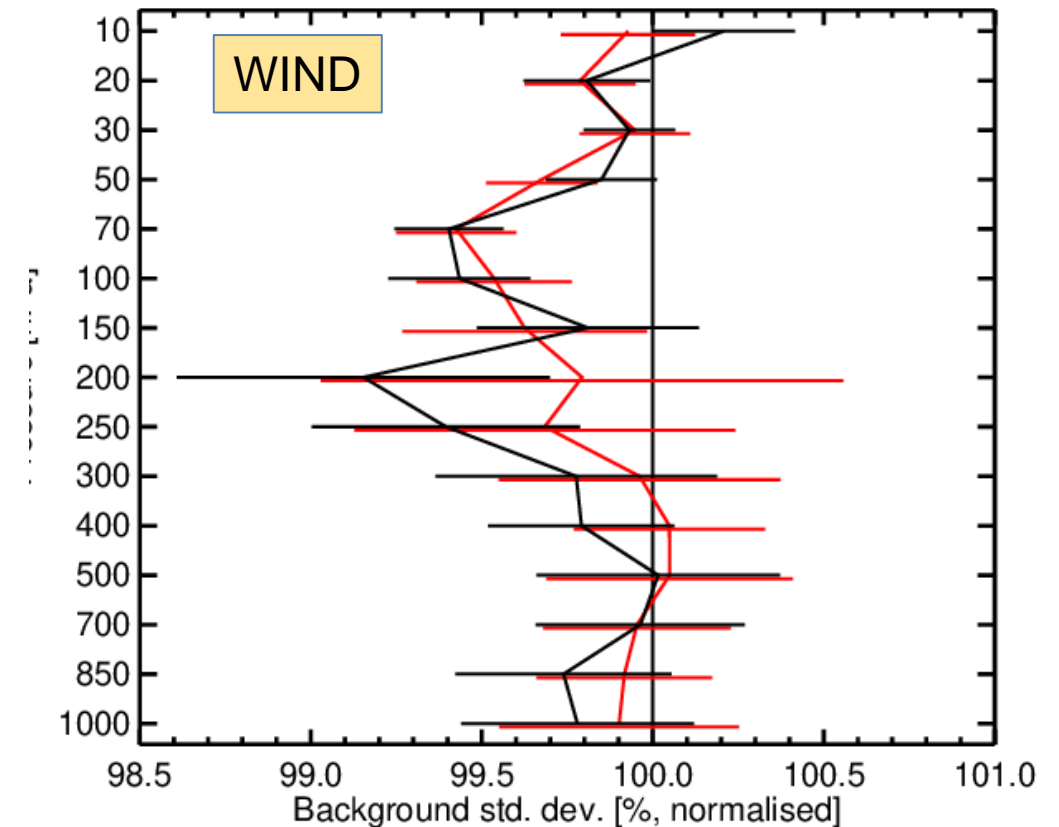
Model Error Estimation and Correction in the IFS: Random errors

Globally-averaged Observation-First Guess StDev norm. diff.

Instrument(s): TEMP – T Area(s): N.Hemis S.Hemis Tropics
From 00Z 16-Jul-2019 to 12Z 22-Aug-2019



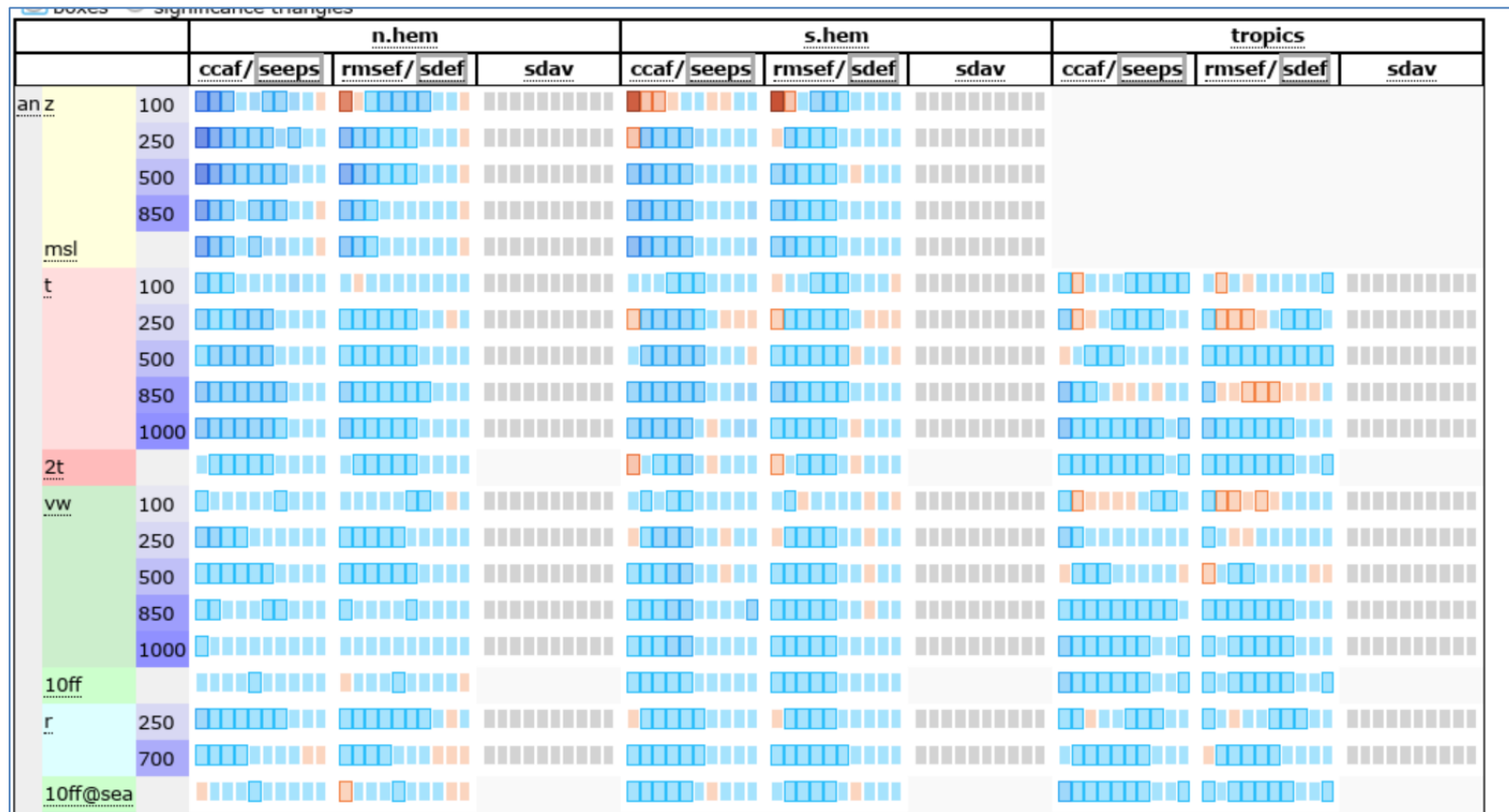
Instrument(s): AIRP PILOT PROF TEMP – U V
Area(s): Europe Japan N.Hemis S.Hemis Tropics
From 00Z 16-Jul-2019 to 12Z 22-Aug-2019



From Bonavita & Laloyaux, 2020

Model Error Estimation and Correction in the IFS: Forecast Skill

- ANN in combination with Weak Constraint 4DVar improves the fit of observations to the model, both in the mean and in the random component.
- What can the ANN bring to **forecast skill**?



Take-home Messages

- Modern ML/DL can be interpreted in the more general framework of Data Assimilation Methodology. While ML/DL is not a conceptual innovation, we can usefully integrate some of its ideas and tools into DA and, more generally NWP/Climate prediction:

“ECMWF will strengthen its leadership position in data assimilation,..., this will include the incorporation of machine learning, with 4D-Var data assimilation being uniquely positioned to benefit from integrating machine learning technologies because the two fields share a common theoretical foundation and use similar computational tools.”

ECMWF Strategy 2021-2030

- ML/DL can have multiple applications in NWP/Climate. Today we have presented ideas and initial results on how to hybridise current DA with ML/DL to either **improve or correct the forecast model inside the Data Assimilation cycle**
- Significant improvements are possible in **analysis accuracy and medium-range forecast skill**. These are initial results and further improvements are expected.

Take-home Messages

- An interesting and open research question is **what happens if we apply the ANN during the forecast** on extended, sub-seasonal, climate scales? To be continued...
- Improving the forecast model(s) is the key challenge to increase predictability from short-range to climate scales. Some in the NWP and Climate communities pin all their hopes on step changes in model resolution, e.g. (sub-)km scale NWP and climate simulations
- Others propose to harness the huge and ever increasing amount of Earth System observations to build completely new models from scratch.
- The **Data Assimilation** approach is to **optimally combine information from both knowledge-based models (at any resolution!) and observation-driven ML models** to find a comprehensively better solution to the problem of estimating the past, current and future evolution of the Earth System

Thanks for your attention!

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Continued...

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