WG3: Model Development, Model Identification, Model Correction, Model Replacement

ECMWF-ESA Workshop on Machine Learning for Earth System Observation and Prediction

Moderators: Massimo Bonavita (ECMWF) and Peter Dueben (ECMWF)

Participants

1. Massimo Bonavita (ECMWF)
2. Peter Dueben (ECMWF)
3. Lucie Rottner (MeteoFrance)
4. Scarlet Stadtler (Juelich Supercomputing Centre)
5. Leyi Wang (Chinese Academy of Sciences)
6. Christian Lessig (University of Magdeburg)
7. Peter Watson (University of Bristol)
8. Weiqi Wan (Chinese Academy of Science)Daniel Ayers (University of Reading)
9. Eliad Bagherzadegan (University of Tehran)
10. Felix Kleinert (Juelich Supercomputing Centre)
11. Giulia Carella (Barcelona Supercomputing Centre)
12. Matthew Chantry (University of Oxford)
13. Michael Langguth (Juelich Supercomputing Centre)
14. Peter Ukkonen (University of Copenhagen)
15. Richard Forbes (ECMWF)
16. Jing-Yi Zhuo (Nanjing University of China)
17. Matej Choma (Meteopress / CTU Prague)
18. Pieter Houtekamer (Environment and Climate Change Canada)
19. Zeng Wu (ETH Zurich)
20. Wenchao Cao (WMO)

Why are participants in the WG interested?

In general:

1. Fascination with the new capabilities
2. Curiosity about ML capabilities and limits
3. Awareness of limitations of conventional tools
4. Interested to see where ML can enhance the workflow
5. What is the trade-off between “classical” approaches (dynamical cores, physical parametrizations) and machine learning / data-driven techniques

Applications:

1. Time series analysis/prediction
2. Model error correction
3. Parameterization emulation
4. Parameterization improvements
5. Replacement of conventional models for short range prediction (eg precipitation, sensible weather param.)
6. Troposphere/Stratosphere dynamics
7. Machine learning to improve predictions for extreme weather
8. Machine learning to improve predictions of tropical cyclones + estimate TC intensity from Satellite pictures
9. Learn machine learning representation of the turbulent flux in boundary layers
10. Real time storm surge simulations with machine learning
11. Machine learning for post-processing

Status and open questions

- *Replace Models...make them faster...improve...where to draw the line?*
  -Hybrid models with dycore and bias correction...we have a lot of data... a bit unclear how much physics we need
  - Hopefully ML can allow for a closer connection between model development and data assimilation

  - Improve the model first… than make it faster
- *Is there a big problem when using ML as black boxes to improve models?*
  - Model development is more complex than just parameter tuning, all-sky data as an example that allows a detailed analysis of test-cases
  - Model error correction potential is clear in DA settings; in forecast settings there are additional caveats but no fundamental reasons why it cannot be useful (a number of groups are looking at this now)
- *Status of physical parametrisation emulation?*
  - A lot of progress has been made but not all issues satisfactorily resolved
  - Parametrisation experts need to be involved more
  - No bigger problem to emulate more very expensive schemes, so expensive schemes should be the (preferred) target
- *Shall we emulate parametrisation schemes individually, or all of them at once?*
  - Maybe use simpler schemes for individual parametrisations and correct for the overall error.
- *Will storm-resolving (km-scale) simulations make a big difference for forecast skill?*
  - It depends what forecast skill you are interested in, but there is little concrete evidence so far.

Status and open questions

- ❖ *How to tradeoff speed and accuracy in emulation? Shall we pick parts of the model that we should emulate based on cost?*
  - Trade-offs between accuracy and speed are very interesting but progress requires an understanding of model uncertainty as you need to know how accurate you need to be
  - Portability to GPUs is also important
- ❖ *How to make sure machine learning models are stable during long integrations?*
  - Crashes in models are a problem with neural networks and they are difficult to tackle in a black box
  - There is still room for improvements
  - Knowledge of the system needs to be combined with machine learning
  - Where do these instabilities come from? not enough data, not the right data, unphysical behaviour
- ❖ *How to add knowledge-based constraints to machine learning?*
  - Develop network architectures that represent physics; introduce constraints to loss function -> ie use the available model as a weak constraint and/or use 1st principles conservation laws as strong constraints
- ❖ *Will machine learning tools help to build more customised products for end-users?*
  - Very likely. Machine learning tools sometimes *beat* existing models and sometimes *enhance* quality of existing models for specific target products
- ❖ *Can a neural networks learn to represent chaotic behaviour (see also discussion below on fuzziness)?*
  - This may be difficult for ML/DL as these are effectively (highly complex/nonlinear) regressions. It has at least partly to do with choice of loss function (ie L2 error norm), we should try to learn from ML/DL solutions in computer vision

Where do you expect ML/DL technology can make the most impact in your area?

- *How to represent model uncertainty in a ML/DL model?*
  -Dropout, Bayesian networks, learn distributions, GANs, re-train an ensemble of models
  -You could also use ML to estimate the uncertainty directly (eg learn a parametrised error distribution)
- *Are we happy with fuzzy results from neural networks?*
  - Depends on whether you want to have a model for the system or whether you want to optimise for a specific model field.
  - More work on loss-function required
  - Train for ensemble-scores and shorter verification tests
  - Weather and climate scientists should define benchmark problems for the ML community.
- *Can we use machine learning to predict extremes? Does more emphasis need to be placed on demonstrating that the methods are improving predictions of extremes?*
  - Would ML be ever able to predict out-of-sample? Depends on the method you use (to learn distributions may be better than NNs).
  - Learn semi-parametric function from data sets
- *Can we train machine learning tools from high-resolution simulations?*
  - This is a very good approach but it requires a sufficient amount of high-resolution data and you will not be able to improve on the most expensive tool: The high-res model!

What are the challenges to realise benefits of Machine Learning?

- ❖ Explainable AI is needed to convince people that machine learning tools are not black boxes (maybe methods to understand what ML is doing are required).
- ❖ Technical challenge to use state-of-the art machine learning tools and to apply them on HPC in order to handle meteorological data which can be huge in size (e.g. high resolution model output).
- ❖ There is a complete disconnect between conventional use of supercomputers (Fortran,MPI,OpenMP) and machine learning (Python...) both for software and hardware. But there will hopefully be some progress soon.
- ❖ Port from tensorflow 1 to tensorflow 2 more difficult than expected/hoped
- ❖ Access to data. This will be a bigger and bigger problem in the future.
- ❖ Not enough independent data points or labelled datasets.
  - Not all petabytes of data avaialble are useful
  - Not clear how to do data augmentation for physical data
  - Transfer learning still at the beginning (e.g. train from CMIP data before training from ERA5 data)