Learning from earth system observations:

Machine learning or data assimilation?

Alan Geer

European Centre for Medium-range Weather Forecasts

alan.geer@ecmwf.int

Thanks to: Massimo Bonavita, Sam Hatfield, Patricia de Rosnay, Peter Dueben, Peter Lean

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Earth system observations

Quantitative methods, e.g. data assimilation

Where physical equations are not known, often qualitative methods, including trial and error

Geophysical analyses

Model development

Improved forecasts and geophysical products

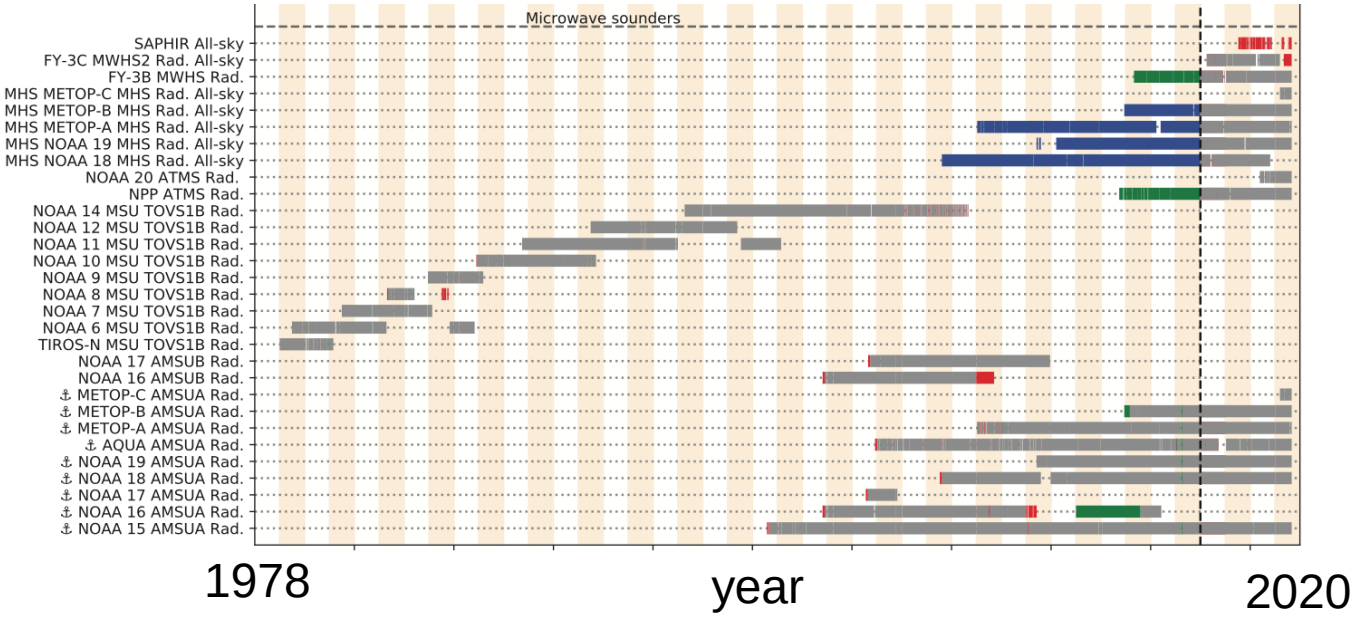
What are the current observational challenges?

Data

Exponential data growth?

About 57,300,000 results

Real earth system observations – actually quite precious



Satellite microwave radiance types assimilated in ERA5

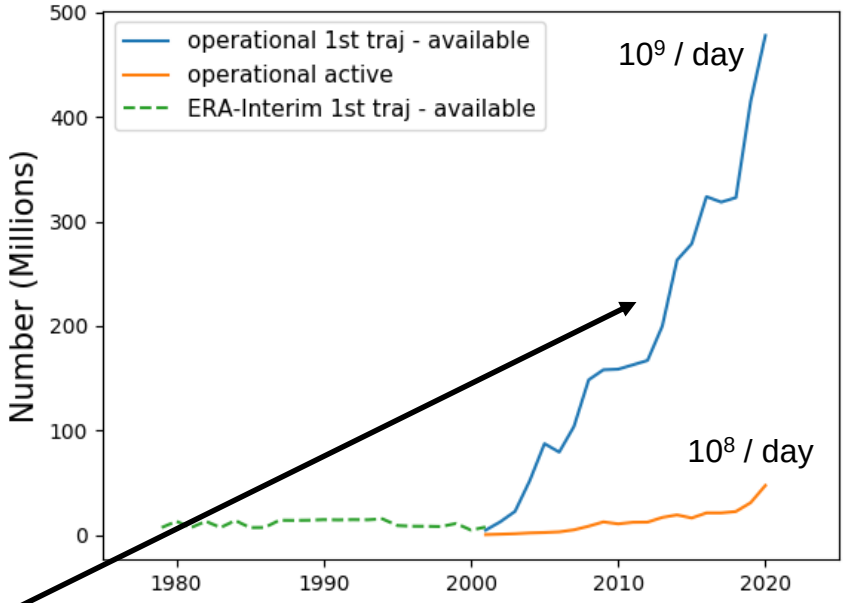
The ERA5 global reanalysis, Hersbach et al., 2020, QJRMetS,
https://doi.org/10.1002/qj.3803

ECMWF

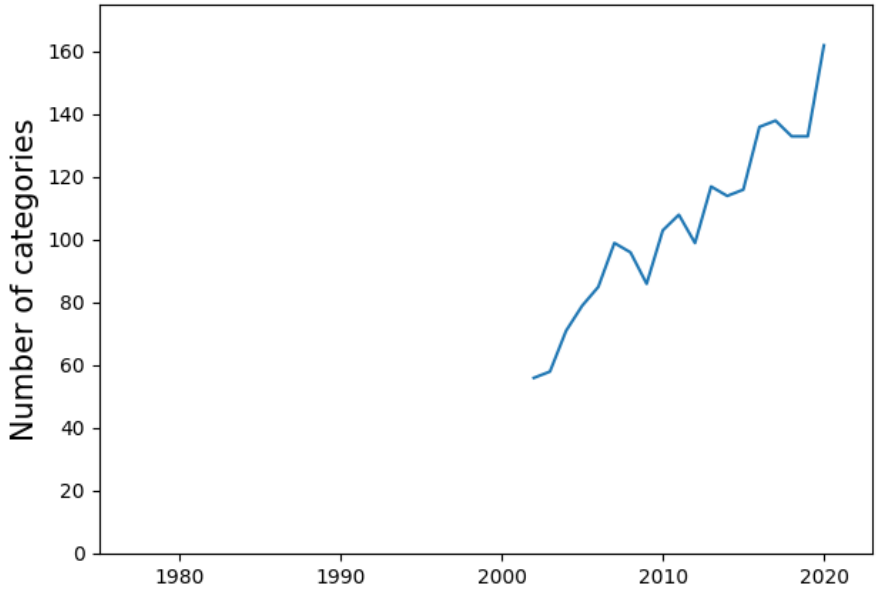
Observation trends at ECMWF – from Peter Lean

Number of observations

Per 12h window



Type of observations



Mostly driven by satellite data:

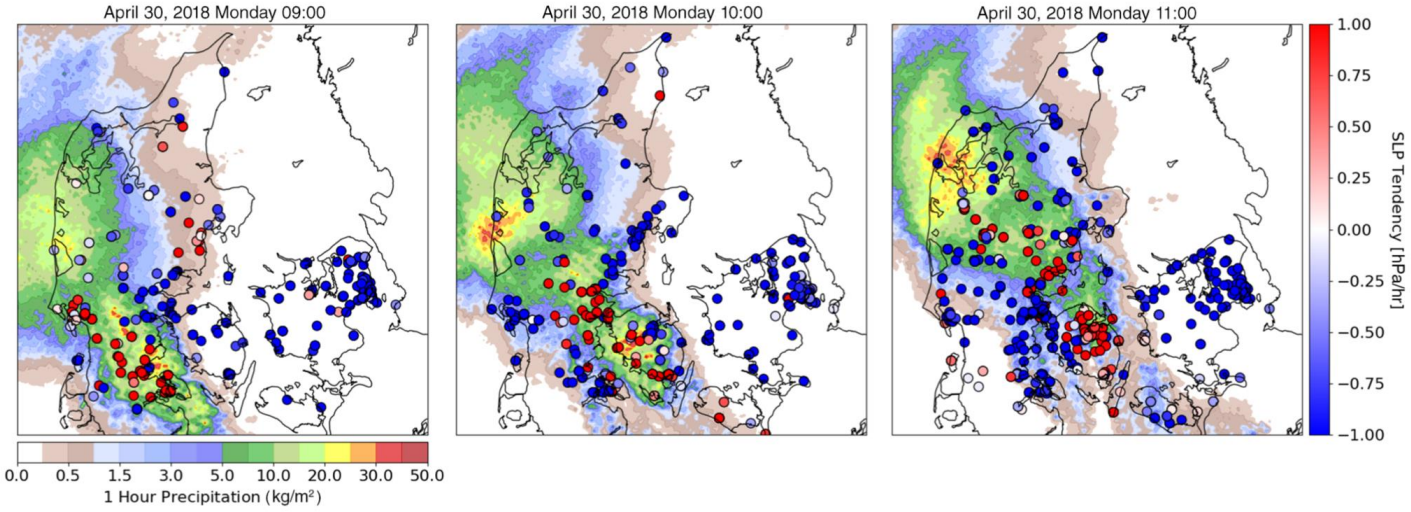
- Move to hyperspectral IR
- Golden age of microwave
- New contributors in the global observing system
- Future: smallsats and constellations

Observation volume increasing (but not exponentially)

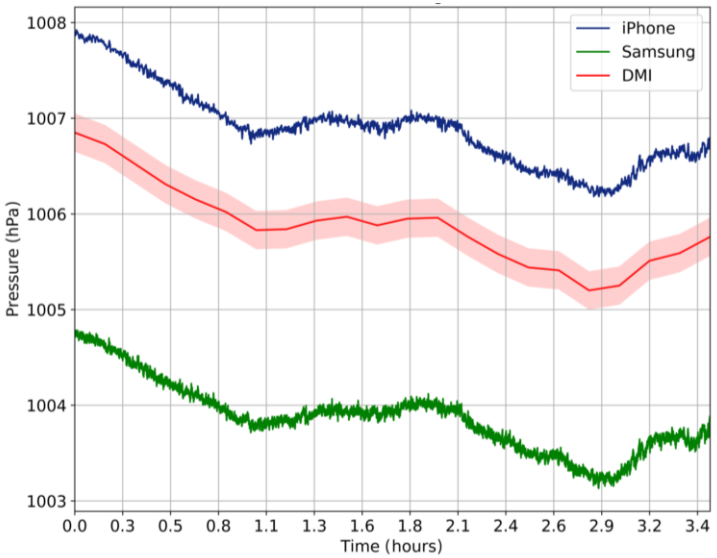
Variety may be a bigger problem

IoT challenges? Example: Smartphone observations

Smartphone pressure tendency (circles) vs. 1h preciptiation



Pressure timeseries



One phone

Barometer

Another phone

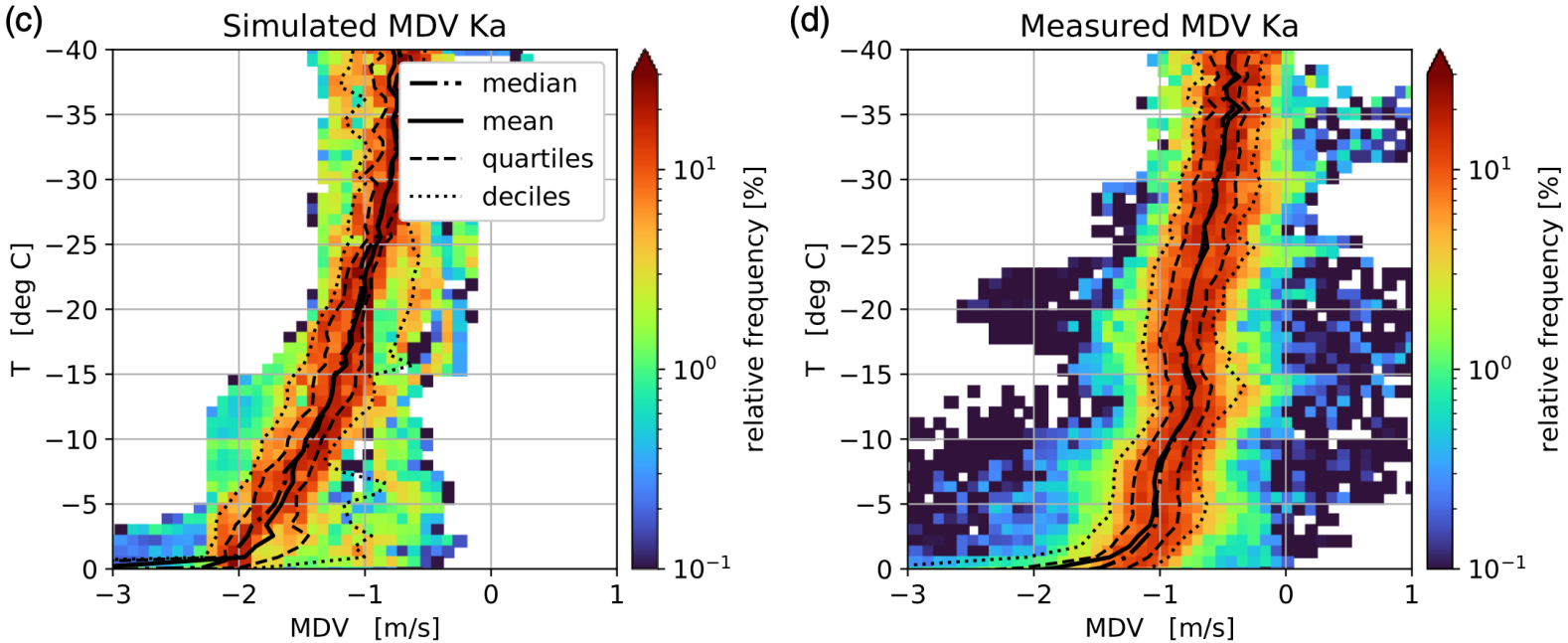
From: Hintz et al. (2019), Collecting and processing of barometric data from smartphones for potential use in numerical weather prediction data assimilation, Met. Appl., https://doi.org/10.1002/met.1805

See also https://www.rmets.org/sites/default/files/2019-10/Hintz_RMetS_Presentation.pdf

IoT challenges: variety, uncertainty, data protection

Observations for model learning: Field sites and campaign data

Mean doppler velocity from 2-month TRIPEx campaign vs. ICON-LEM simulations

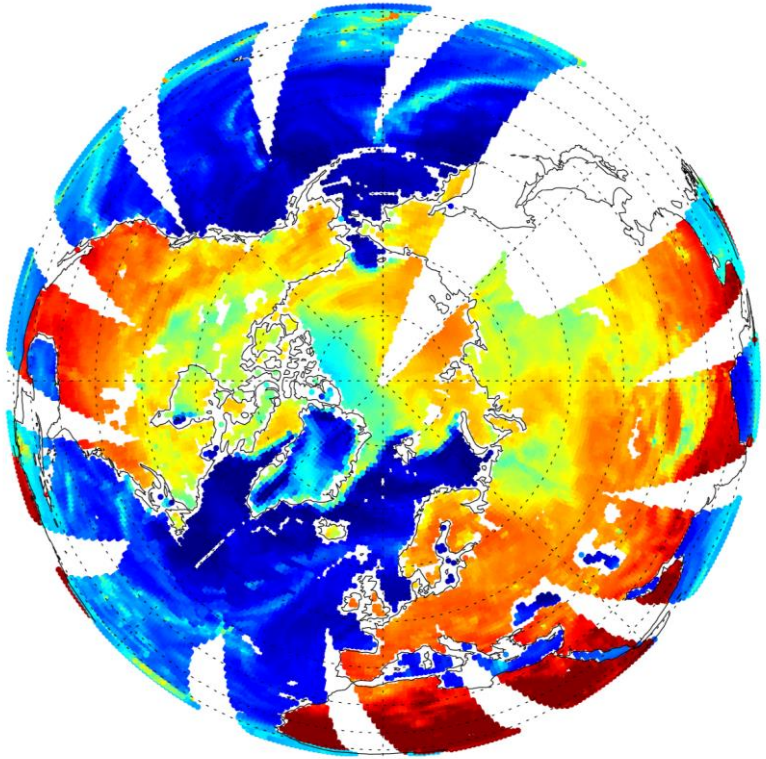


From: Ori et al. (2020) Evaluation of ice particle growth in ICON using statistics of multi-frequency Doppler cloud radar observations, QJRMetS, https://doi.org/10.1002/qj.3875

These kind of highly heterogeneous observations need to be brought into the global observing system

Real observations: sparse, uncertain, **ambiguous**

Satellite observations



SSMIS F-17 channel 13 (19 GHz, v)
Microwave brightness temperatures
3rd December 2014

$$y = h \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_{\ldots} \end{pmatrix}$$

Forward function

Geophysical variables

Atmospheric temperature, water vapour, wind, cloud, precipitation

Skin and substrate temperature and moisture

Ocean wind, waves, foam

Sea-ice

Snowpack

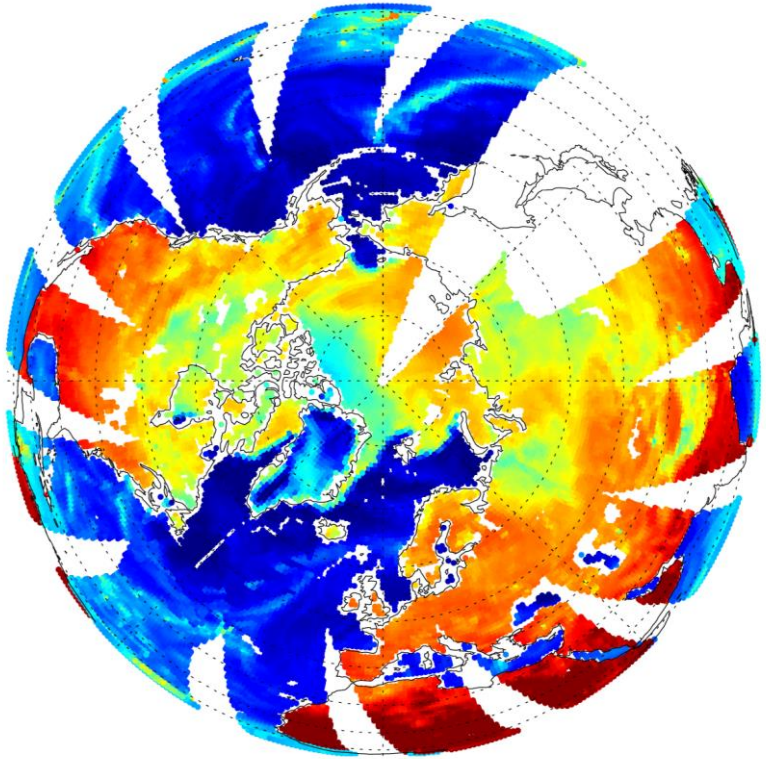
Ice

Vegetation

Soil

Real observations: sparse, uncertain, **ambiguous**

Satellite observations



SSMIS F-17 channel 13 (19 GHz, v)
Microwave brightness temperatures
3rd December 2014

Geophysical variables

Equations & parameters – where sometimes knowledge is quite uncertain

$$y = h\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_{\ldots} \end{bmatrix}, \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_{\ldots} \end{bmatrix}\right)$$

Forward function

Gas spectroscopy

Scattering from hydrometeors

Cloud and precipitation micro and macro-structure

Snow / ice grain size and structure

…..

Varied, sparse, uncertain, ambiguous observations

→ Bayesian inverse methods

→ Data assimilation

ECMWF

The forward and inverse problem

Forward model

Observations

$$y = h(x, w)$$

Geophysical state

Model parameters

$$\cancel{x, w = h^{-1}(y)}$$

Inverse model

No unique solution: ill-posed

The best that observations can do is to provide a statistical improvement in our knowledge of x and w

The inverse problem solved by Bayes theorem

Observations

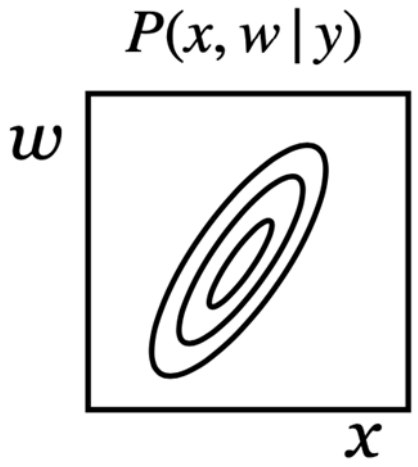
Geophysical state

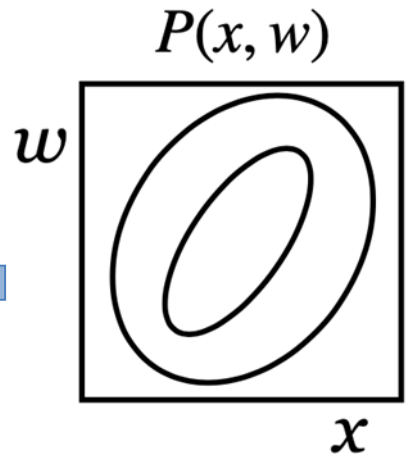
Model parameters

Bayes theorem

$$P(x, w|y) = K\ (y, P(y|x, w), P(x, w))$$

Probabilistic equivalent of the forward model h()





(Posterior) Probability of x and w given y

Prior probability of x and w

Cost function for variational DA

Assume Gaussian errors (error standard deviation σ)
and for clarity here simplify to scalar variables
and ignore any covariance between observation, model or state error

variety, ambiguity, sparsity

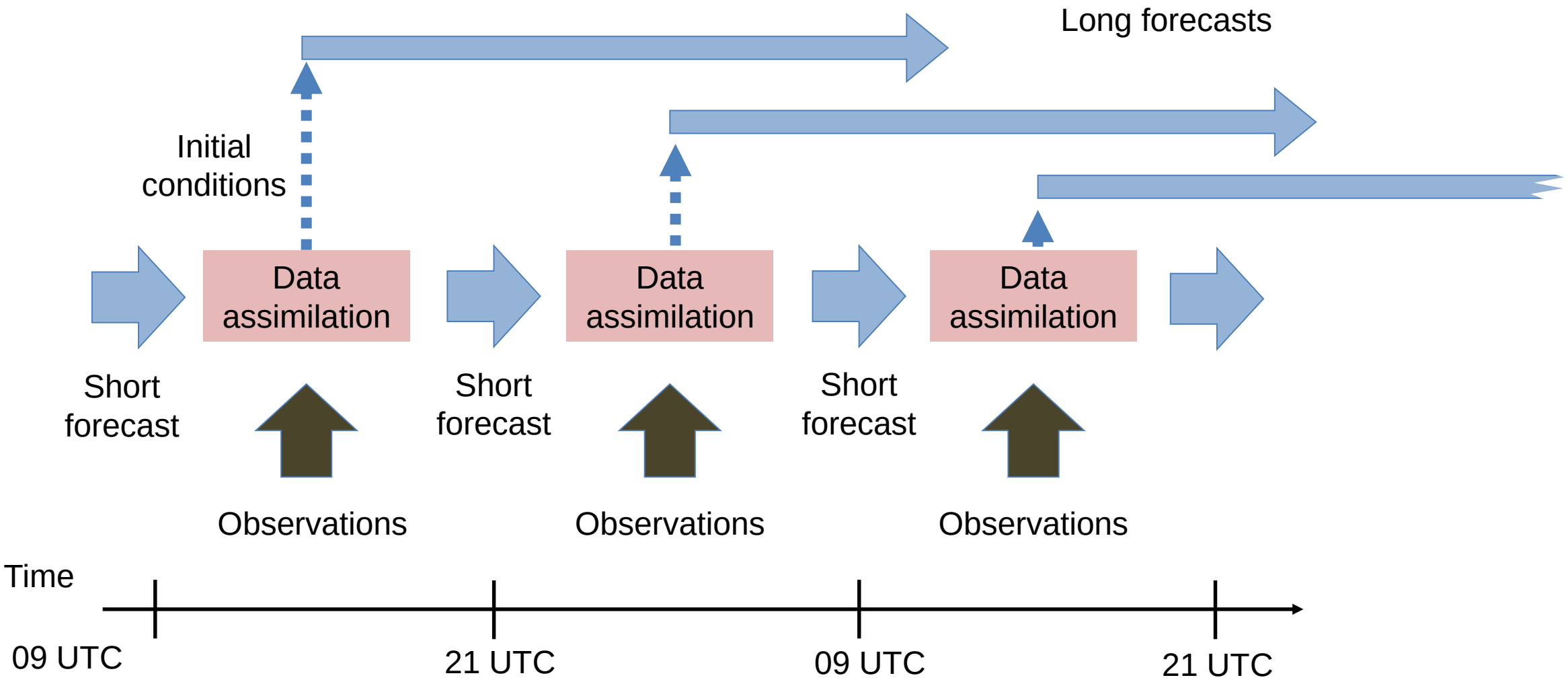
uncertainty

$$J(x,w) = \underbrace{\frac{(y-h(x,w))^2}{(\sigma^y)^2}}_{J^y} + \underbrace{\frac{(x^b-x)^2}{(\sigma^x)^2}}_{J^x} + \underbrace{\frac{(w^b-w)^2}{(\sigma^w)^2}}_{J^w}$$

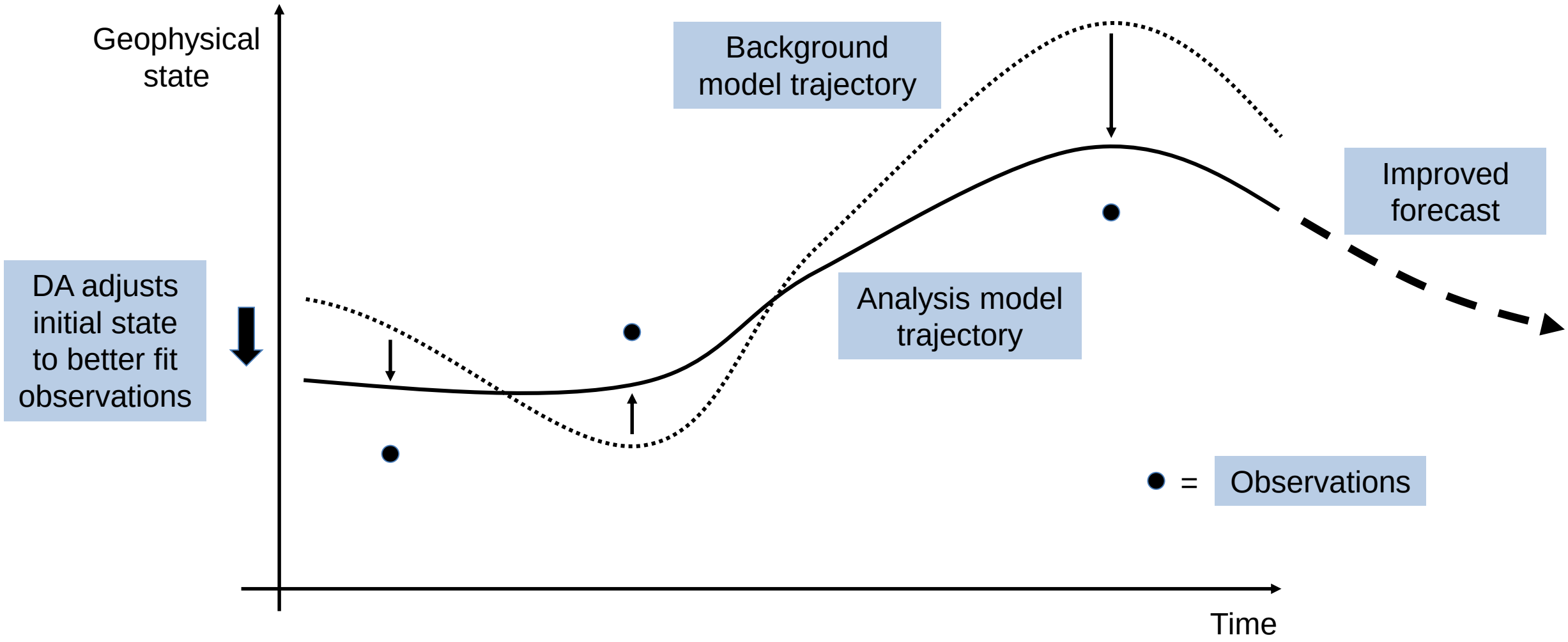
DA | Cost function | Observation term | Prior knowledge of state | Prior knowledge of model

Data assimilation for numerical weather prediction: (NWP)

Blending short forecasts and new observational data in a statistically optimal way



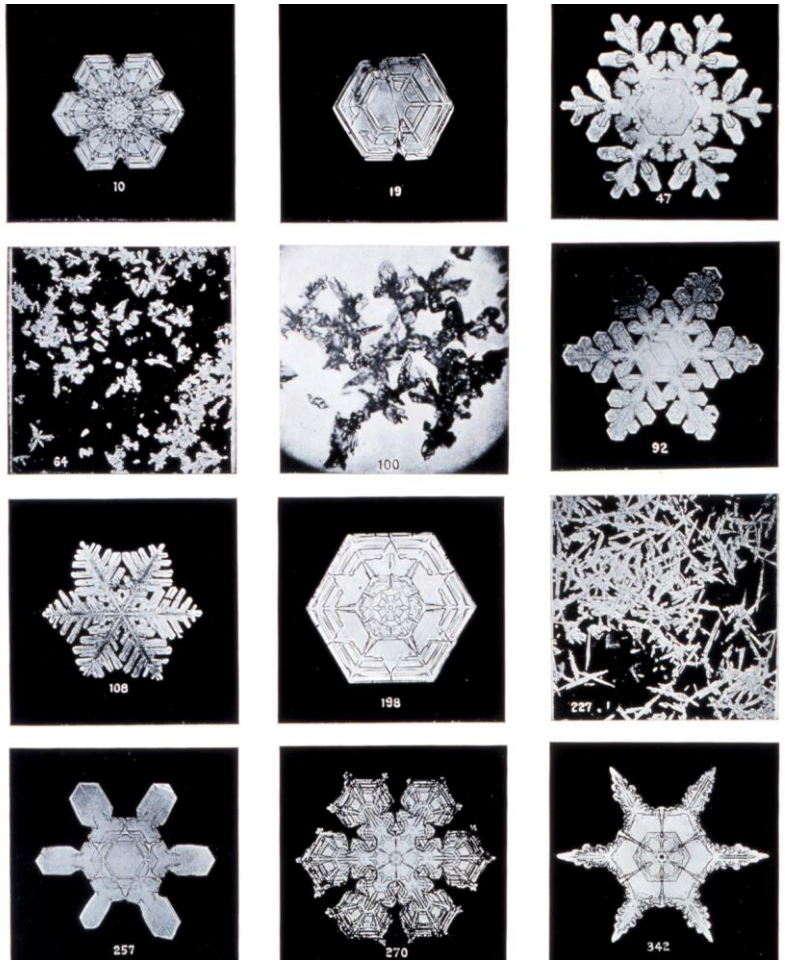
4D-Variational DA with a **perfect model assumption**



But models are not perfect…

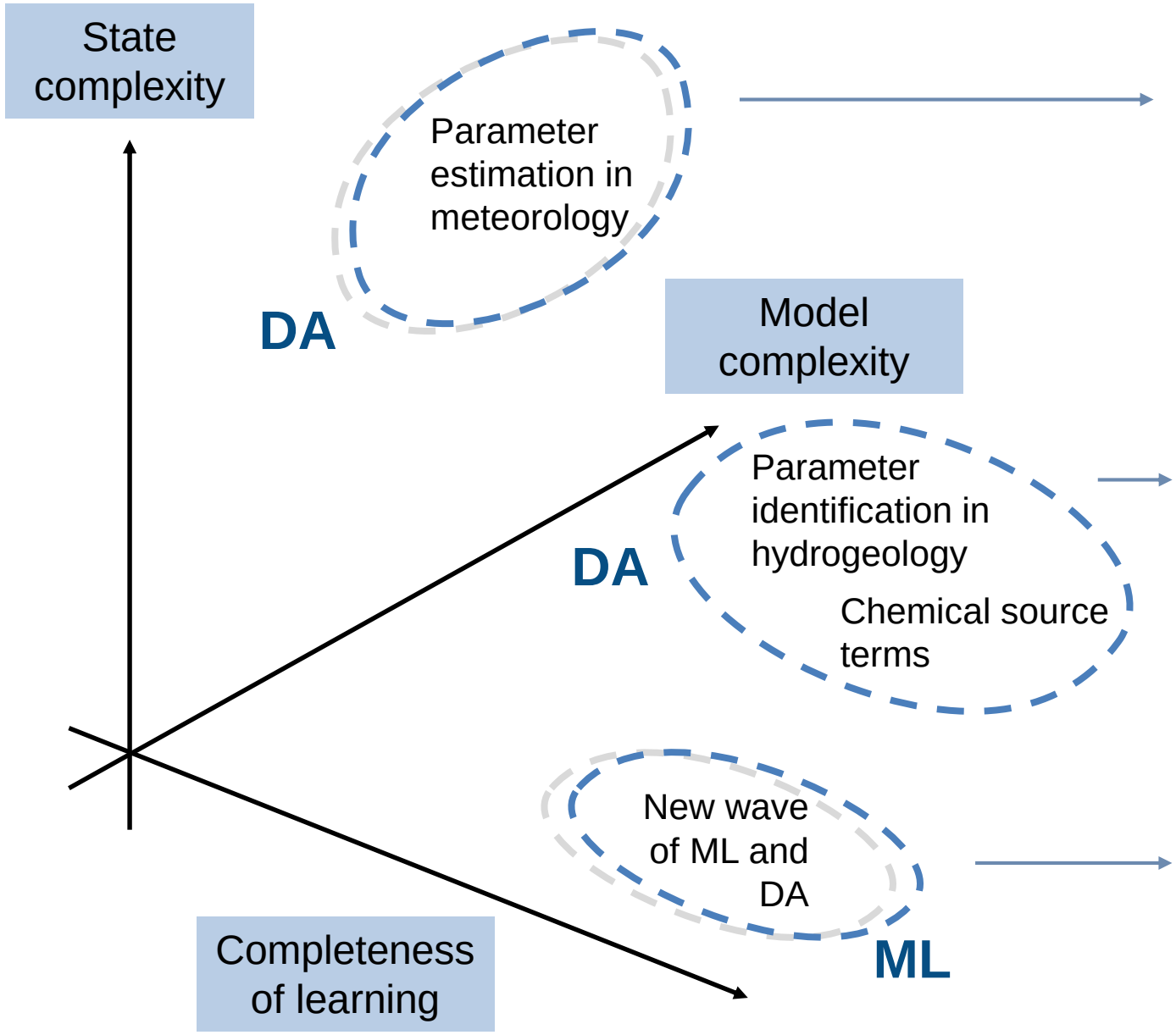
- Within the fluid systems (atmosphere / ocean):
  - Truncation of model resolution and dynamical processes (e.g. 8 km currently) therefore needing parametrisations of diffusion, turbulence, gravity waves etc.
  - The water problem: phase changes
    - Cloud and preciptiation processes – microscopic scales
    - Sea-ice

- Throughout the earth system – many processes or boundary conditions that are not modeled from physical first principles and/or are strongly heterogeneous in time and space
  - Biosphere, lithosphere, aerosols ...



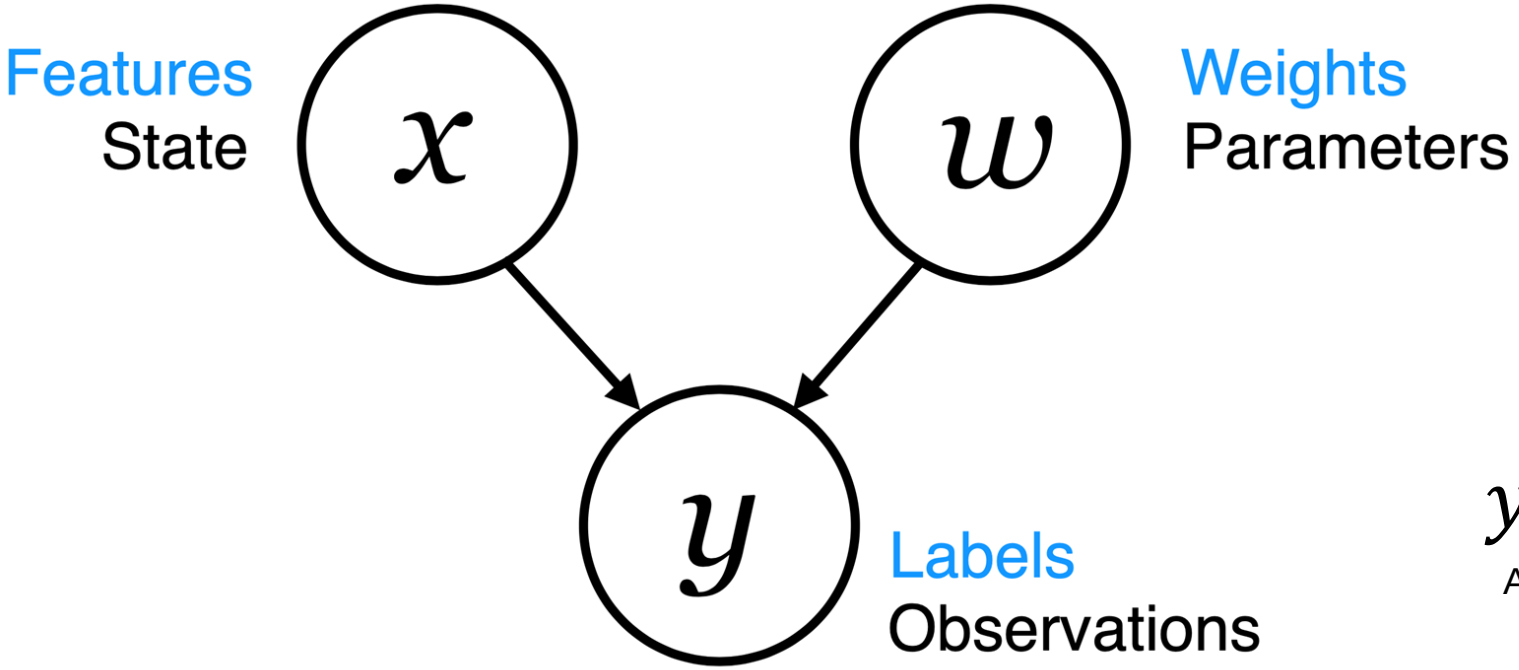
Wilson Bentley (1902, http://www.photolib.noaa.gov)

Model learning from observations



- Simultaneous state and parameter estimation:
  - Autoconversion parameter learnt in a GCM (Kotsuki et al., 2020) https://doi.org/10.1029/2019JD031304
  - Roughness length learnt in local area model (Ruckstuhl and Janjić, 2020) https:/doi.org/10.1175/MWR-D-19-0233.1
- Pure parameter estimation, e.g:
  - Groundwater modeling, e.g. hydraulic conductivity (Zhou et al., 2014). https://doi.org/10.1016/j.advwatres.2013.10.014
  - CO_2 source term estimation (Peylin et al., 2013) https://doi.org/10.5194/bg-10-6699-2013
- Model (and sometimes) state estimation in simple models:
  - ML of KS equation (Pathak et al., 2018) https:/doi.org/10.1103/PhysRevLett.120.024102
  - Use DA to infer ODE representation of Lorenz models (Bocquet et al., 2019) https://doi.org/10.5194/npg-26-143-2019

Bayesian equivalence of ML and DA



$$y = h(x, w)$$

As a Bayesian network

Geer (2020) https://doi.org/10.21957/7fyj2811r

Bocquet et al. (2020) https://arxiv.org/abs/2001.06270

Abarbanel et al. (2018) https://doi.org/10.1162/neco_a_01094

Hsieh and Tang (1998) https://doi.org/10.1175/1520-0477(1998)079%3C1855:ANNMTP%3E2.0.CO;2

Goodfellow et al. (2016) https://www.deeplearningbook.org

Cost / loss function equivalence of ML and variational DA

Assume Gaussian errors (error standard deviation σ)
and for clarity here simplify to scalar variables
and ignore any covariance between observation, model or state error

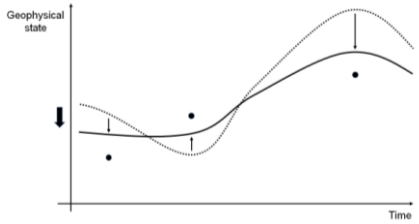
ML — Loss function

Basic loss function — Feature error? — Weights regularisation

$$J(x,w) = \underbrace{\frac{(y-h(x,w))^2}{(\sigma^y)^2}}_{J^y} + \underbrace{\frac{(x^b-x)^2}{(\sigma^x)^2}}_{J^x} + \underbrace{\frac{(w^b-w)^2}{(\sigma^w)^2}}_{J^w}$$

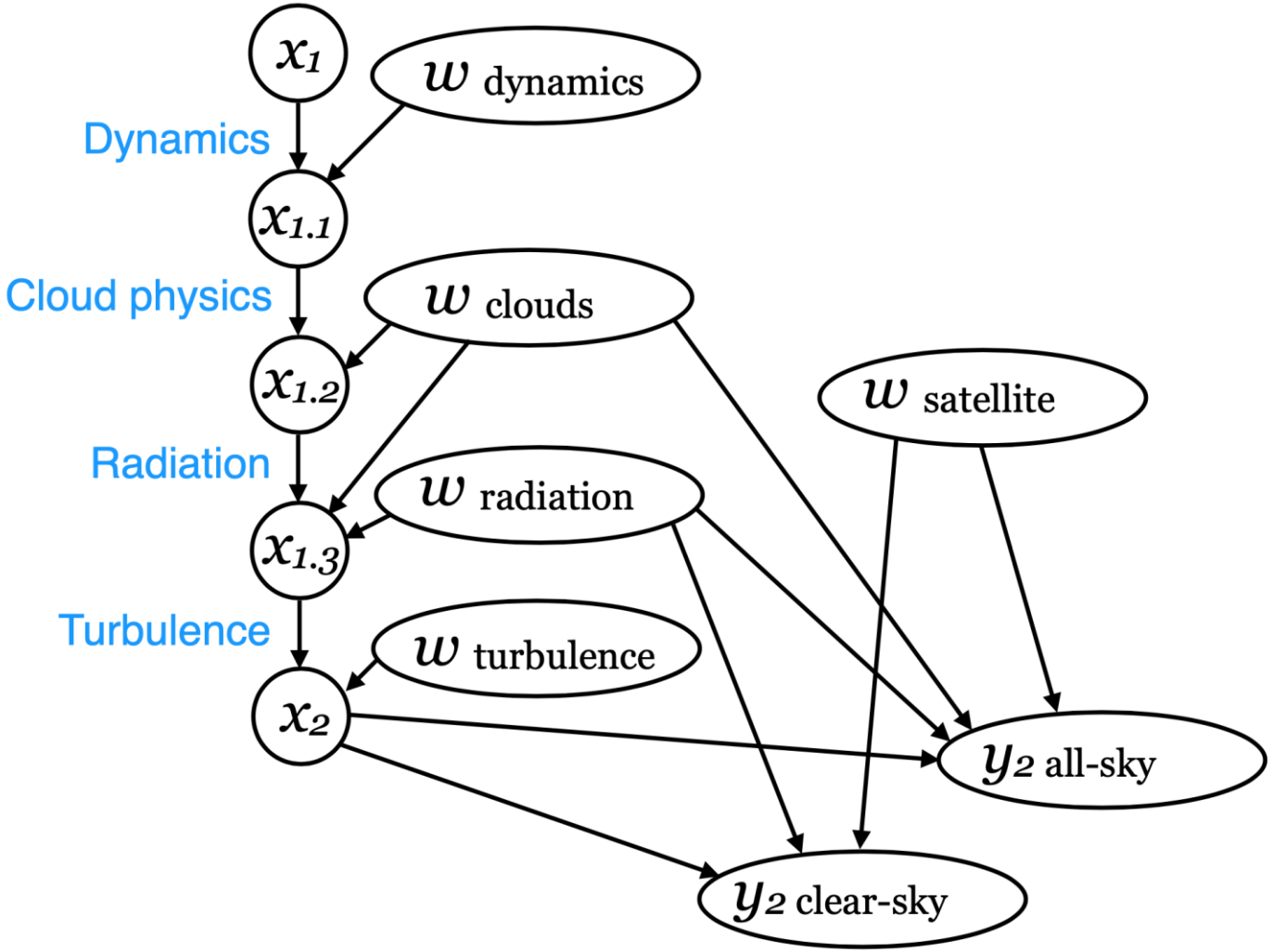
DA — Cost function

Observation term — Prior knowledge of state — Prior knowledge of model

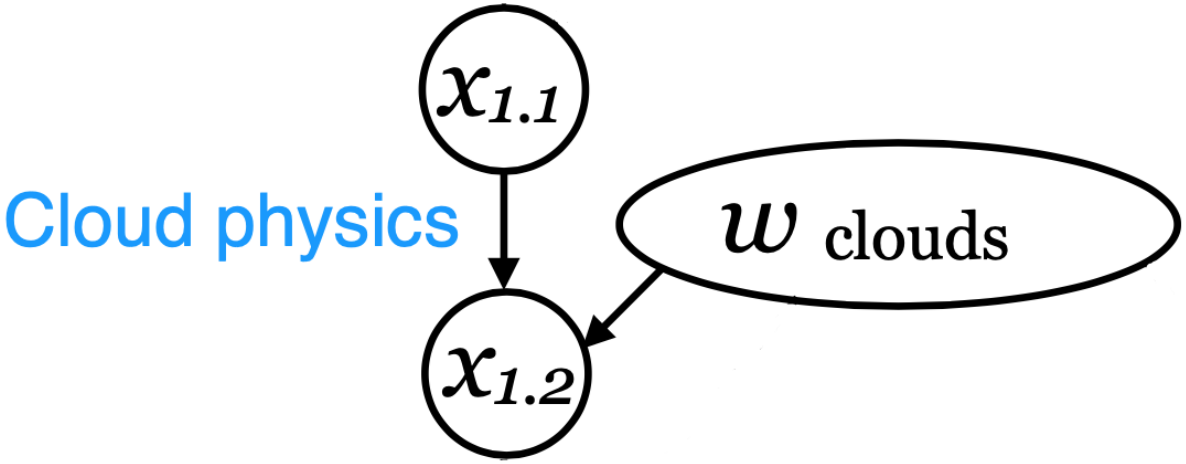


Inside an atmospheric model & data assimilation timestep

One model time-step

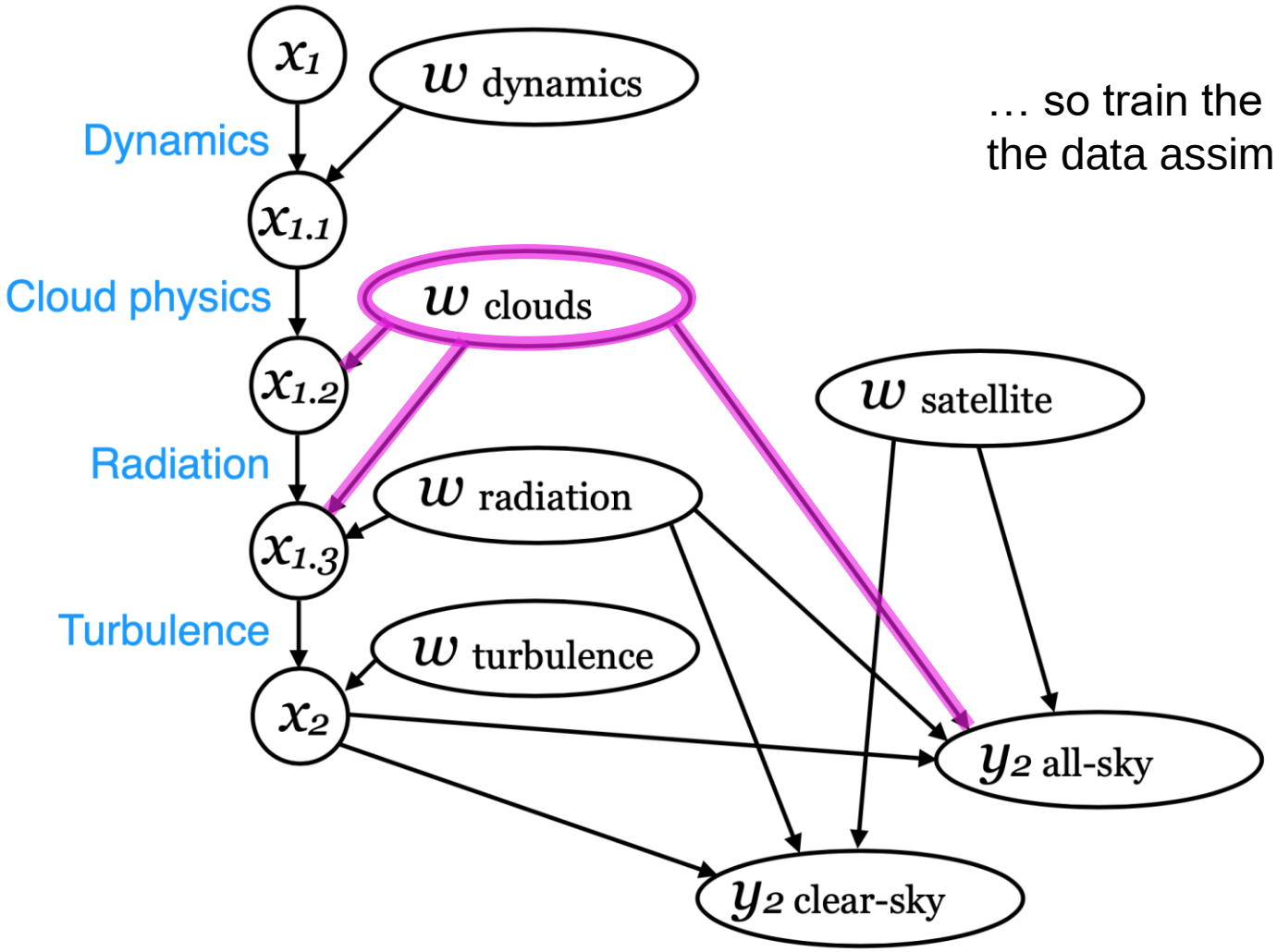


Learning an improved model of cloud physics (ML or DA)



We want to train a model against observations, but we cannot directly observe gridded intermediate states $x_{1.1}$ and $x_{1.2}$ … or more precisely model tendencies …

Inside an atmospheric model



… so train the model inside the data assimilation system

Snow micro- and macro-physical parameter estimation (Geer, 2020, submit AMT?)

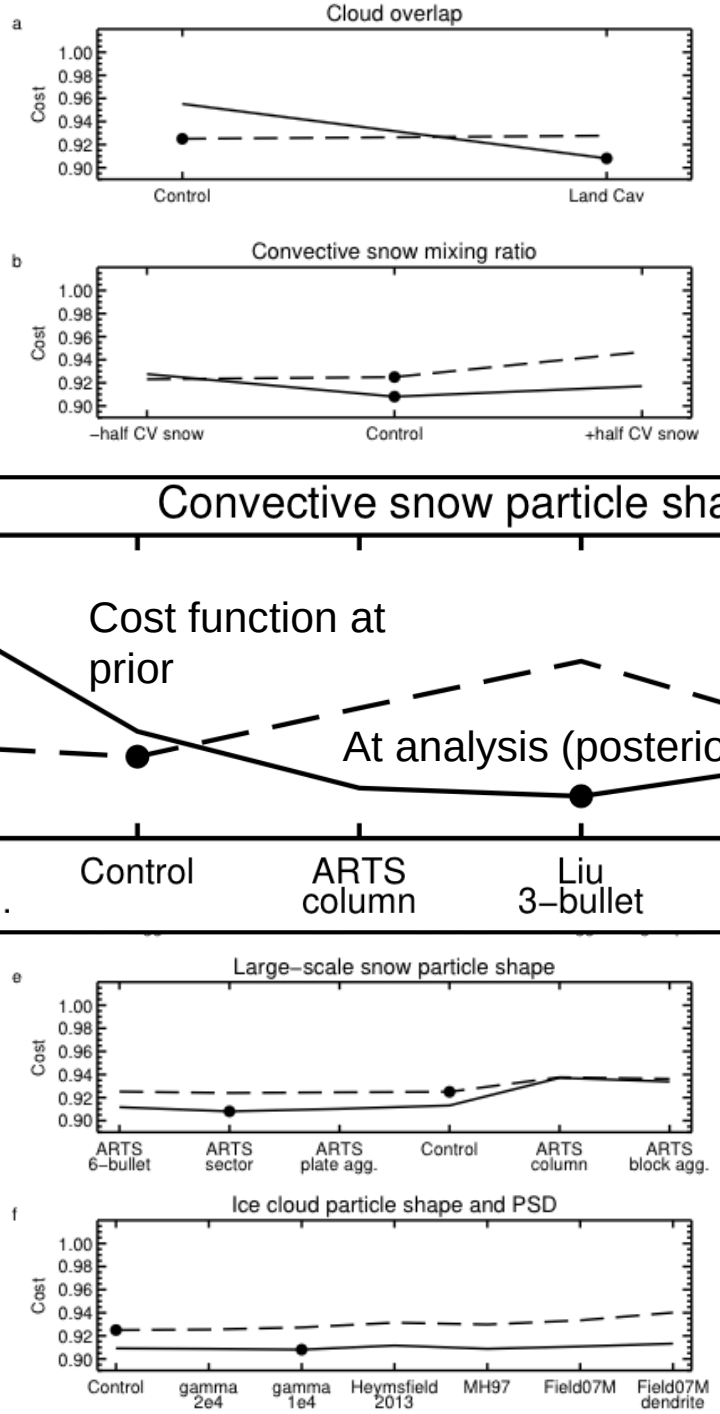
Offline physical parameter search

- cost function between ECMWF model and SSMIS observations
- 6 parameters from RTTOV-SCATT radiative transfer model

Issues:

- Cost function has multiple minima
- Cost function is based on mapped mean and skewness, not the squared error (errors are highly non-Gaussian)
- Some aspects are quite ambiguous (e.g. snow mixing ratio versus particle shape)

See also e.g. Posselt and Bishop (2012)
https://doi.org/10.1175/MWR-D-11-00242.1



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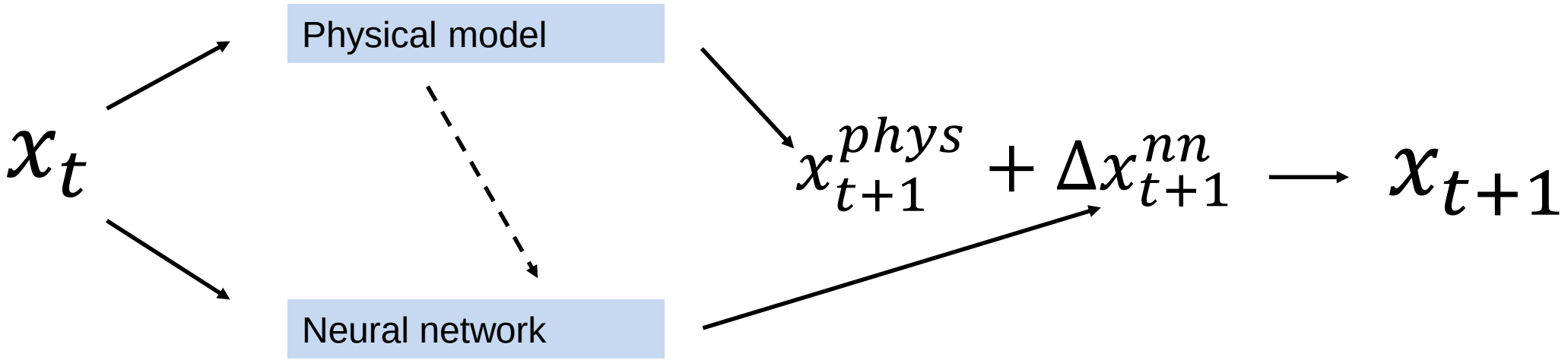
Ultimate goal: state and model learning, direct from observations, in real time

→ But first, more achievable ideas

ECMWF

Learning model error

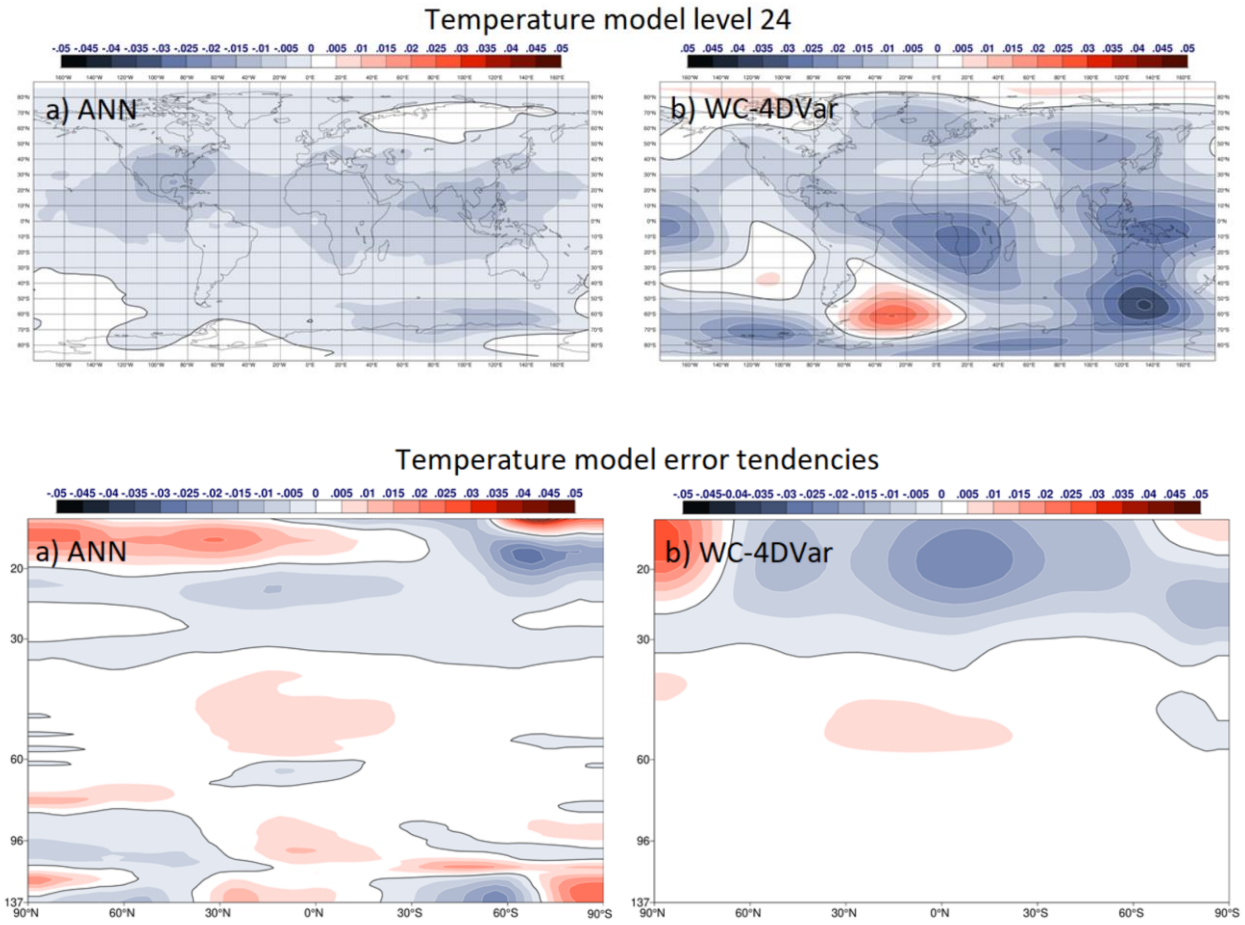


e.g.
Physics guided neural networks (lake temperature): Karpatne et al. (2018) https://arxiv.org/abs/1710.11431
Uresolved scale learning: Brajard et al. (2020) https://arxiv.org/abs/2009.04318

Model error correction using ML – Bonavita and Laloyaux (2020, submitted to JAMES, https://www.essoar.org/doi/abs/10.1002/essoar.10503695.1)

Offline ML – learn weights w of model for model error tendency

$$J(x,w) = (y - h(x,w))^2$$



Weak-constraint 4D-Var, done online (w is a field of model error tendencies)

$$J(x,w) = \ldots + \frac{(w^b - w)^2}{(\sigma^w)^2}$$

Where can ML techniques help improve DA applications in the earth sciences?

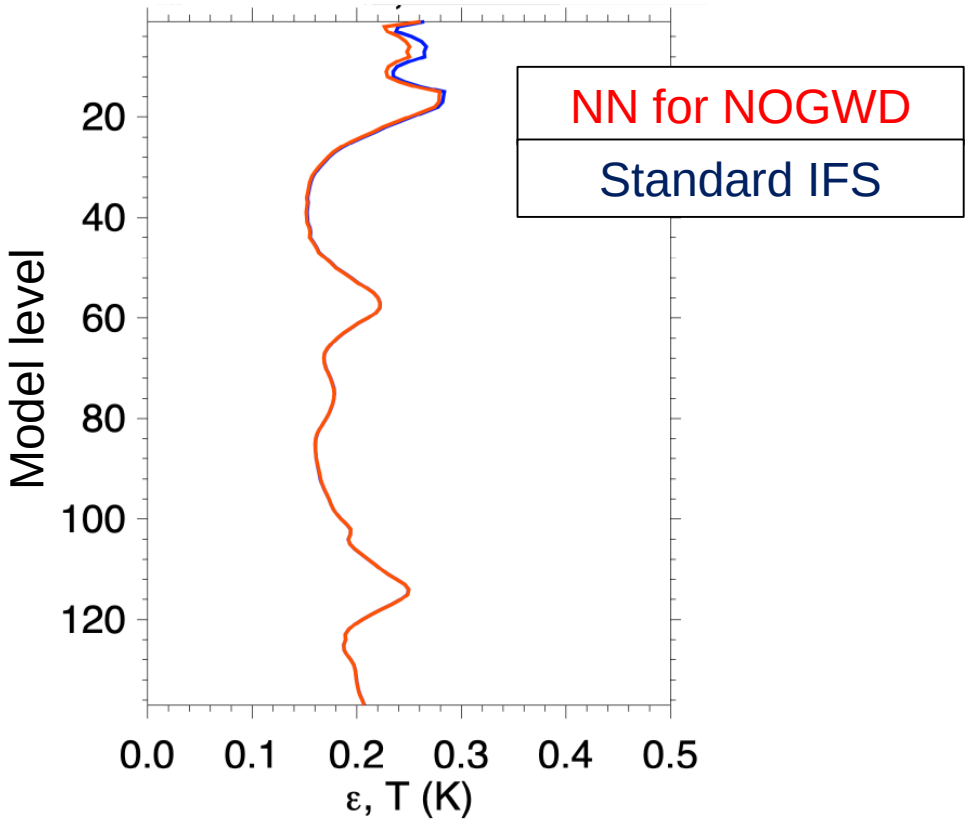
- Hybrid DA – ML (e.g error learning)
- ML as a statistical accelerator or surrogate model for inverse methods:
  - In Monte-Carlo inverse frameworks (e.g. ensemble DA, particle filtering, Markov Chain Monte Carlo)
    - E.g. Calibrate – Emulate - Sample (Cleary et al., 2020) https://arxiv.org/abs/2001.03689
  - In variational frameworks (e.g. 4D-Var)
    - Accelerate the differentiation of the cost function (upcoming slide)
- ML as a modelling component where physical models are lacking
  - E.g. observation operators for surface-sensitive observations
- Dozens of other possibilities (see: this workshop + NOAA AI workshop)

Automatic differentiation for variational DA tangent-linear and adjoint operators:

Hatfield, Chantry et al. (ongoing work)

- Train a NN on IFS non-ographic gravity wave drag scheme (NOGWD)
- Differentiate the NN via the chain rule to get:
  - TL (tangent-linear)
  - Adjoint (== back-propagation)
- Use the NN TL and adjoint in the 4D-Var (but keep the physical nonlinear NOGWD scheme)
  - Succesful 2-month run of IFS cycling 4D-Var completed

48h TL test of full IFS forecast model



$$\varepsilon = \langle |\mathrm{H}\delta x - h(x+\delta x) - h(x)| \rangle$$

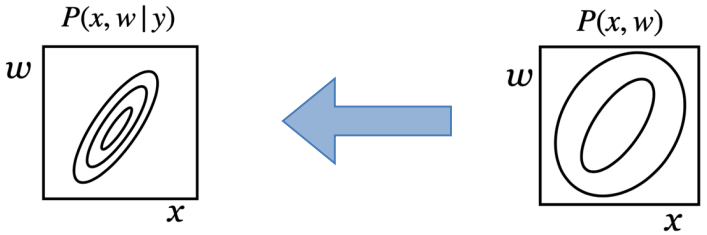
Tangent linear model

Nonlinear model

Could DA techniques and the Bayesian approach help improve ML in earth sciences?

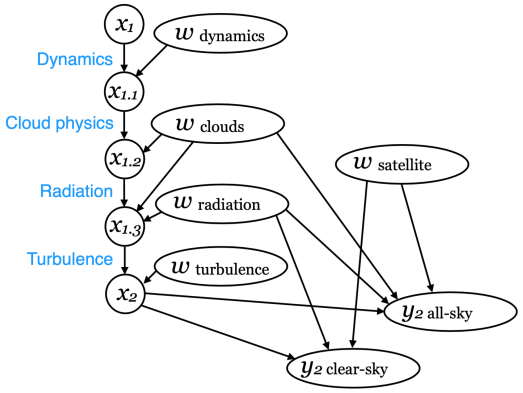
- Can data normalisation be replaced with a more quantitative physical description of label and feature uncertainty?
  - In the same way DA quantifies observation and background error matrices

Bayesian perspective: treat all variables as probabilistic and represent any prior knowledge probabilistically too



- Use physical layers:
  - As an output layer, physical observation operators can move from gridded geophysical states to observation space
  - Physical constraint layers to take advantage of prior knowledge where it exists (e.g. known physical laws)

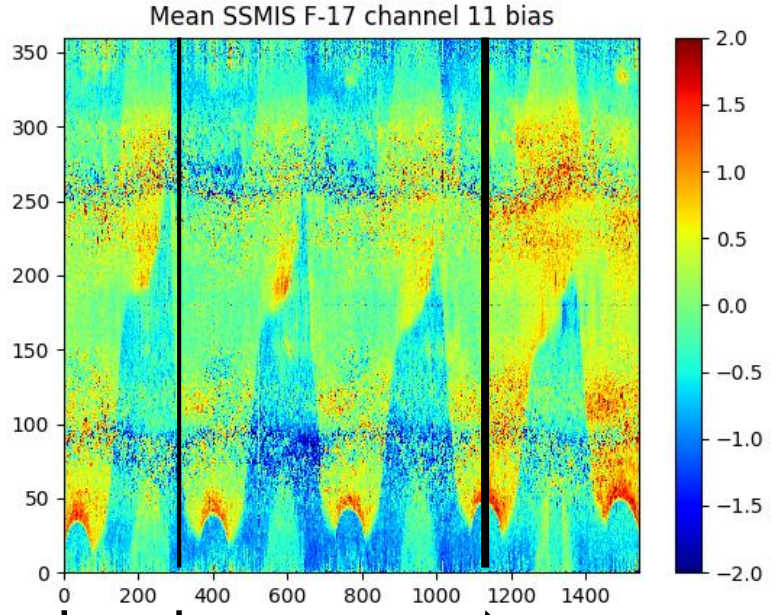
Bayesian perspective: constrain solution using prior physical knowledge (embedded in physical models)



Satellite bias correction using ML

- Application: SSMIS instrument solar-dependent calibration anomalies
- Offline training of a bias model in observation space
  - Learn bias between observations and model as a function of satellite-solar orbital parameters.
- Problems: many latent variables, orbit changes, model changes

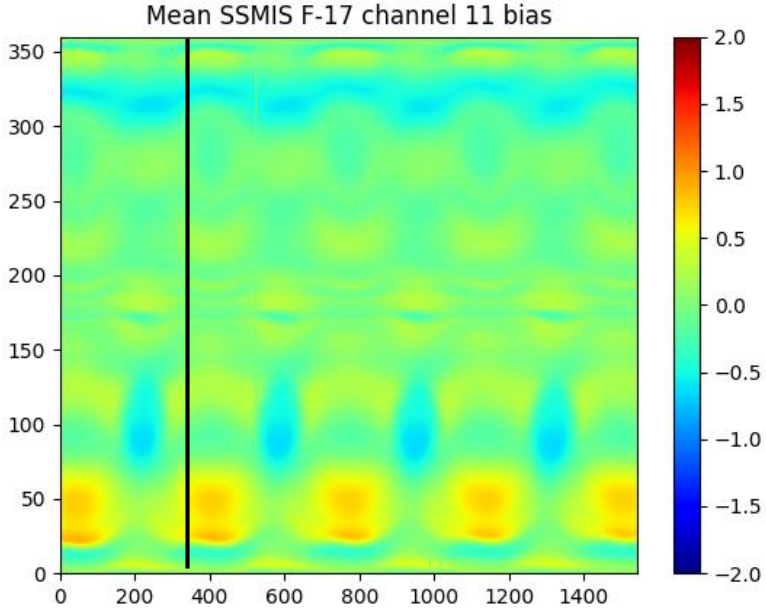
Daily binned bias



Training set: 360 days

Model upgrade

Static NN model predicted

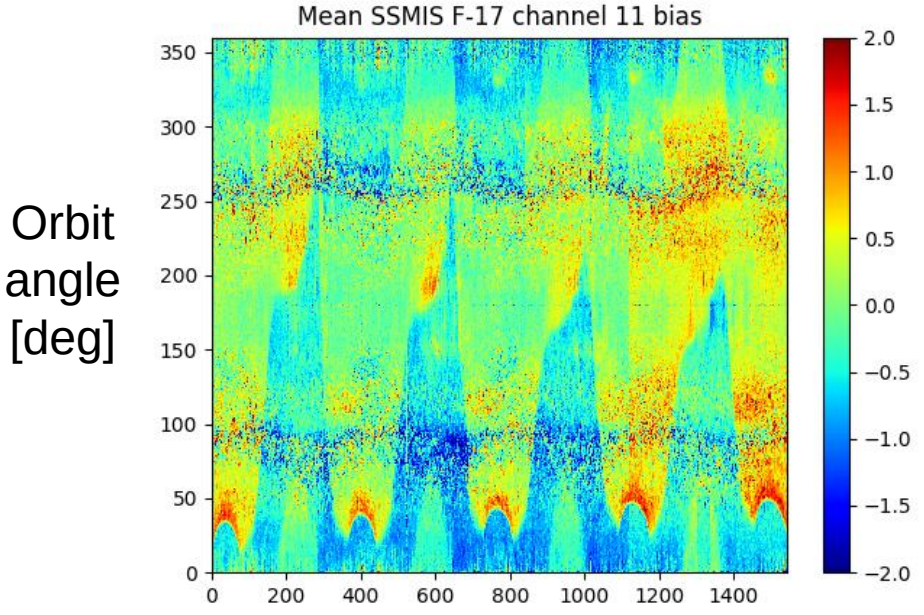


Bias [K]

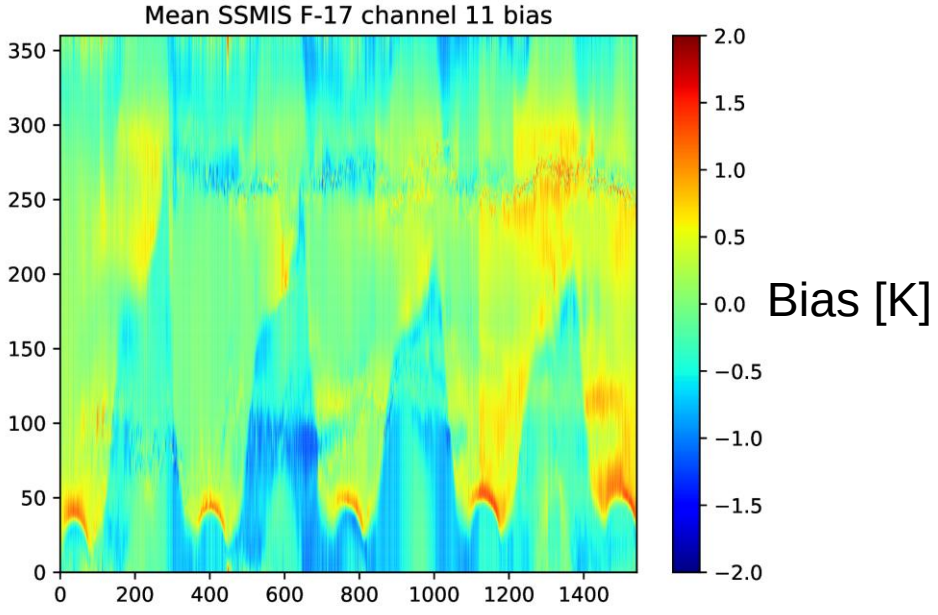
Satellite bias correction

- Dynamic NN approach:
  - Re-train each day on yesterday's biases
  - Learn bias as a function of orbit angle
- This is essentially an offline, nonlinear version of VarBC, which is a standard bias correction technique for DA

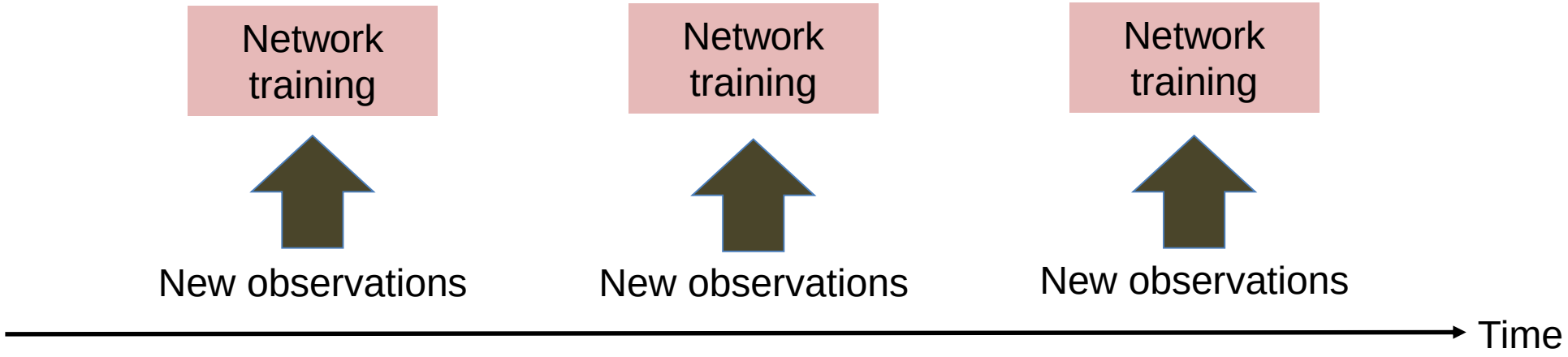
Daily binned bias



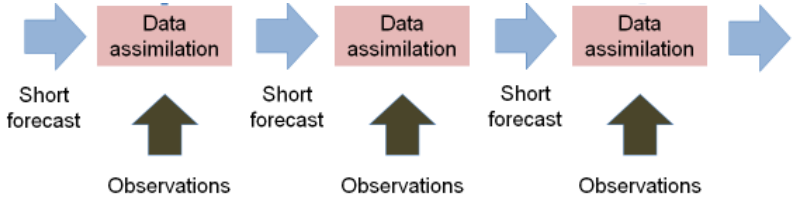
Dynamic NN model predicted



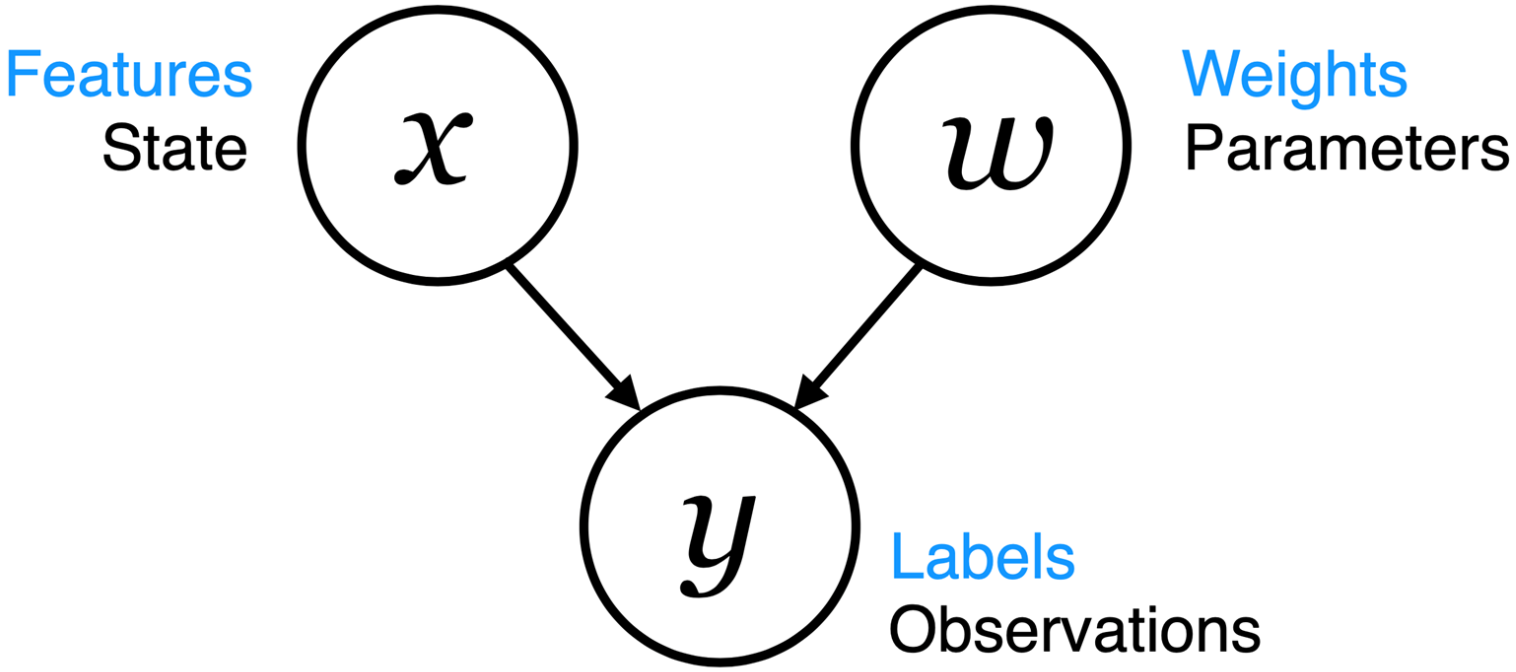
Sequential learning



- Batch learning
  - relearn on everything, i.e. past and new data, each time?
  - take pre-trainined network and run training on new data only
- Sequential learning
  - e.g. Online sequential Extreme Learning Machine (OS-ELM, Liang et al., 2006) https://doi.org/10.1109/TNN.2006.880583
  - e.g. Forecasting daily streamflow using OSELM (Lima, Cannon, Hsieh, 2016) https://doi.org/10.1016/j.jhydrol.2016.03.017
- How close are these techniques to the overarching Bayesian framework, i.e. to data assimilation?



Bayesian equivalence of ML and DA → hybridise DA ML → just Bayesian inverse methods



Summary

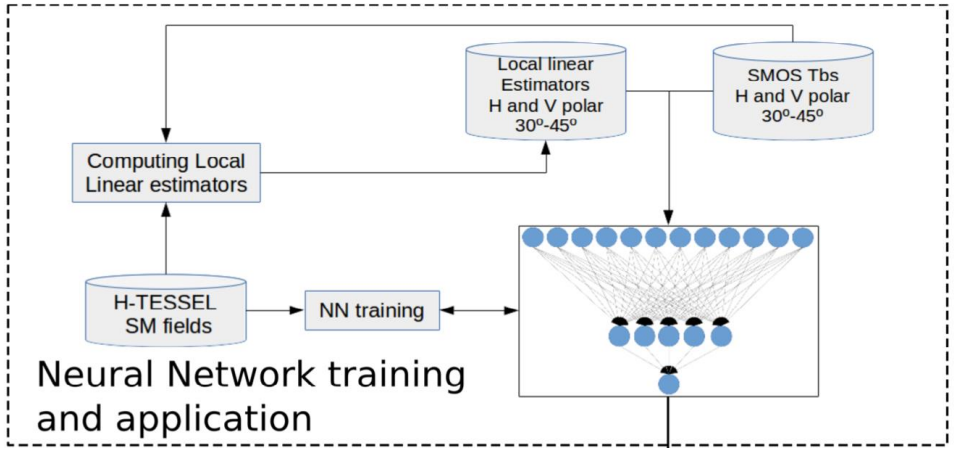
- Observational challenges
  - Real observations are diverse, sparse, ambiguous, uncertain but precious – we are not overwhelmed!
  - Data assimilation arose exactly to deal with diverse, sparse and indirect observations
- Model learning from real observations
  - Hybrid DA – ML to supersede existing approaches?
- DA to benefit ML?
  - More physical, more Bayesian (e.g. explicit error representations, physical constraint layers)
- ML to benefit DA?
  - Surrogate models for speeding up inference
  - Learned model components where physical models are unavailable

Extras

Observation operators using ML

- Fast observation operators (e.g. radiative transfer operators RTTOV and CRTM) are already ‘ML’ – just using linear regression or heuristic model components
  - Train on physical reference models
  - Train directly between model background and observations

- E.g. Soil moisture
  - Single hidden layer NN trained between SMOS observations and model soil moisture (H-TESSEL or IFS)
  - A version of this is used in the operational ECMWF forecasting system



Rodriguez-Fernandez, N., de Rosnay P., Albergel C., Richaume P., Aires F., Prigent C., Kerr Y.: "SMOS Neural Network Soil Moisture Data Assimilation in a Land Surface Model and Atmospheric Impact", Remote Sensing, 11(11), 1334, 2019
https://www.mdpi.com/2072-4292/11/11/1334

Time evolution of state