

Data assimilation and machine learning

Alan Geer

European Centre for Medium-range Weather Forecasts

alan.geer@ecmwf.int

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Thanks to: Matthew Chantry, Marcin Chrust, Massimo Bonavita, Sam Hatfield, Patricia de Rosnay, Peter Dueben



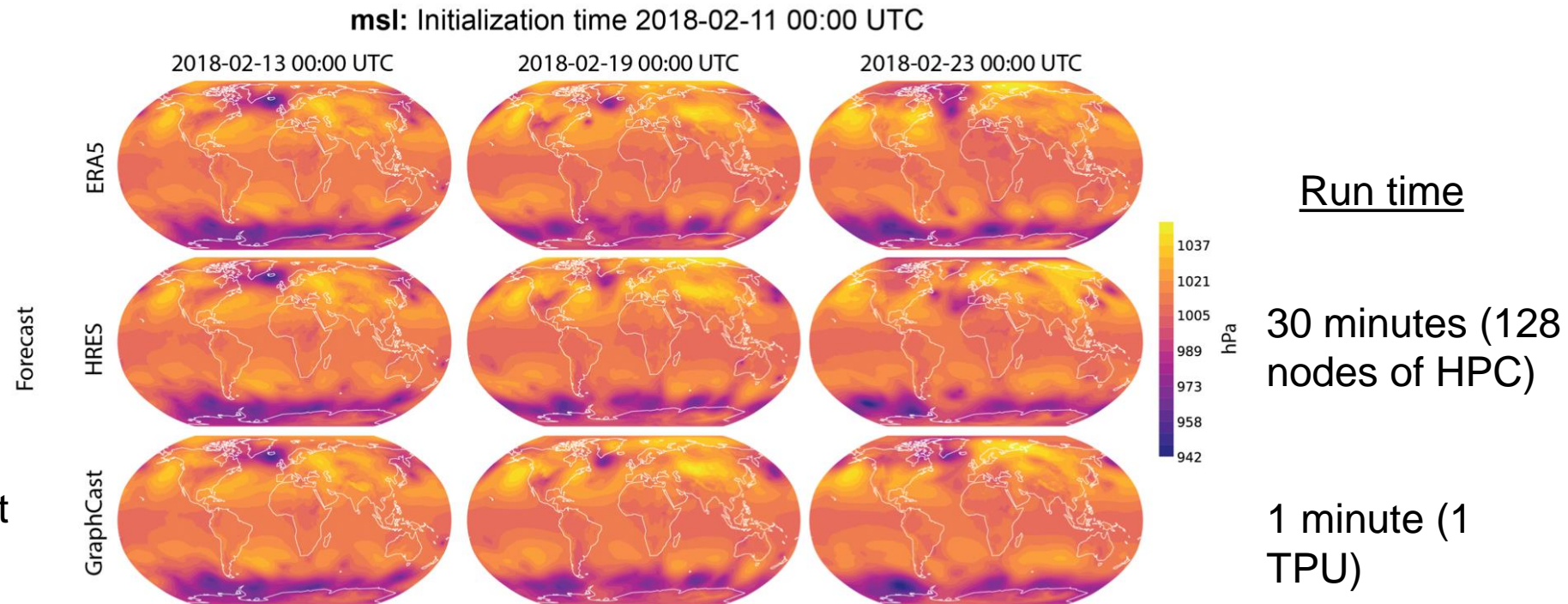
Forecast models based on machine learning are here and they're good!

- Huawei's Pangu-Weather (Bi et al., 2022, *arXiv preprint arXiv:2211.02556*)
- Google DeepMind's GraphCast (Lam et al., 2022, *arXiv preprint arXiv:2212.12794*)

ERA5: reanalysis as **training data (1979-2017)** and validation data (2018)

HRES: ECMWF T1279Co (9 km) 10 day forecast

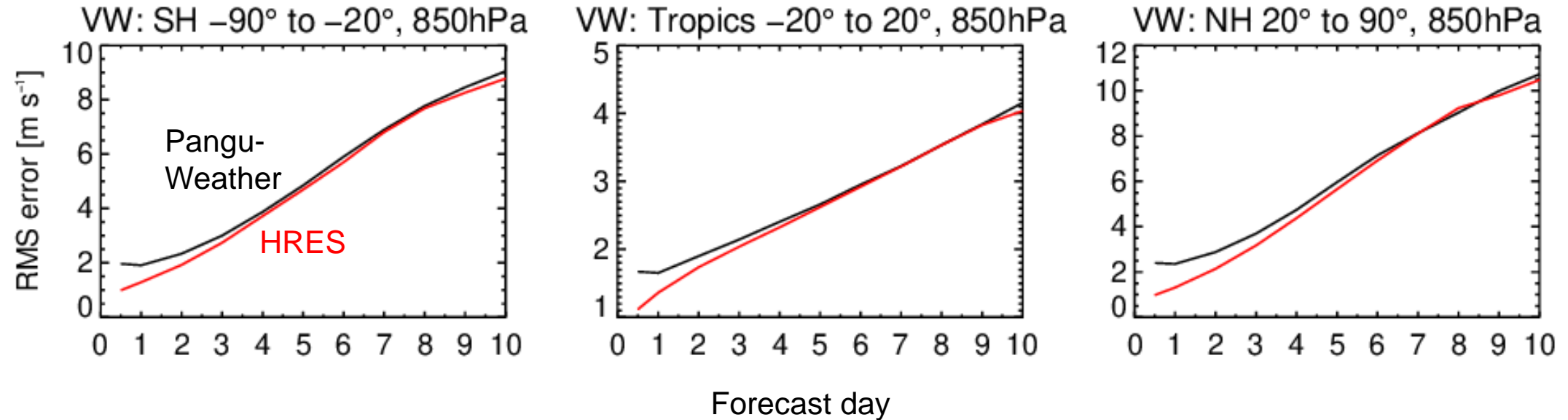
GraphCast: 10 day forecast at 0.25 degrees (25 km)



<https://arxiv.org/pdf/2212.12794.pdf>

RMS vector wind error of operational forecasts: ML vs. ECMWF HRES

Pangu-Weather running from ECMWF operational analysis (credit: Mat Chantry, Huawei, ECMWF colleagues)



Should we start making forecasts by ML, not physics?

- Full geophysical validation and testing of ML forecasts is ongoing:
 - Smoothness, physical consistency between variables? High impact weather?
- ML only provides a limited subset of outputs (due to cost of training and forecasting an ML model to cover the full product range of NWP)

	GraphCast	Pangu-Weather	ECMWF HRES	
Horizontal res	25 km	25 km	8-9 km	10x higher
Vertical levels	37	13	137	4-10x higher
Upper air parameters (prognostic)	6 Z/Q/T/U/V/W	5 Z/Q/T/U/V	7 Z/Q/T/U/V/L/I/C	Also prognostic cloud 2x higher
Upper air diagnostic	0	0	9 E.g. rain, snow	
State size	2×10^8	7×10^7	$\sim 10^{10}$	
Timestep	6h	1h	7.5 minutes	8x higher

In total HRES has ~1000x more outputs. And full HRES is needed for DA

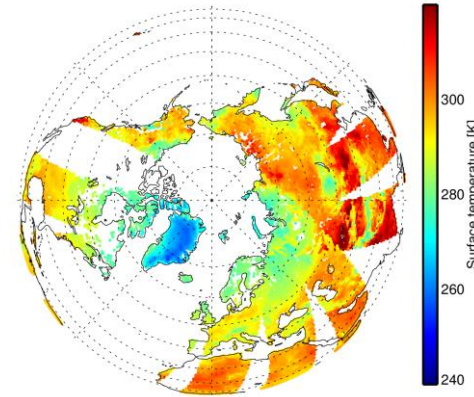
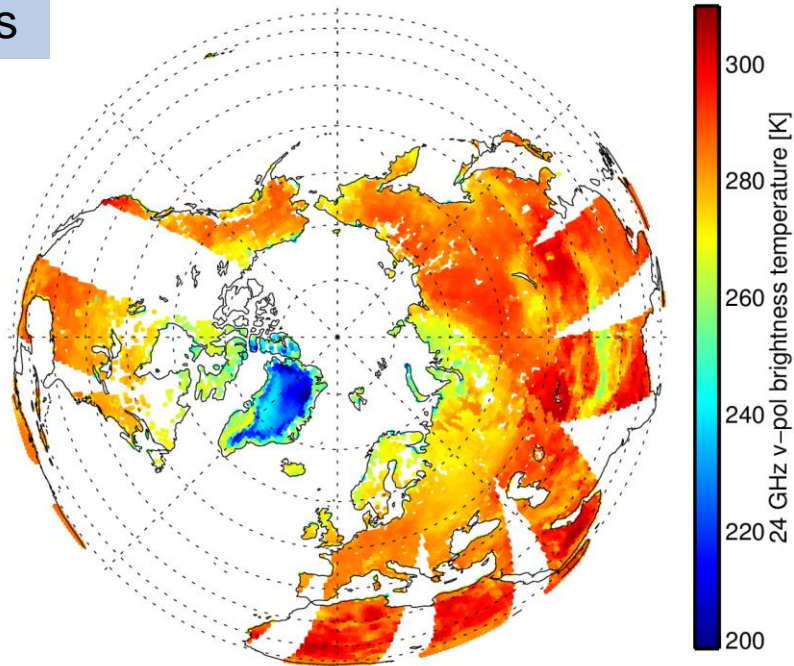
An ML example: microwave land surface observation operator

Python, Keras, Tensorflow, Numpy, Matplotlib, Xarray

Datasets

AMSR2 24GHz v-pol observations

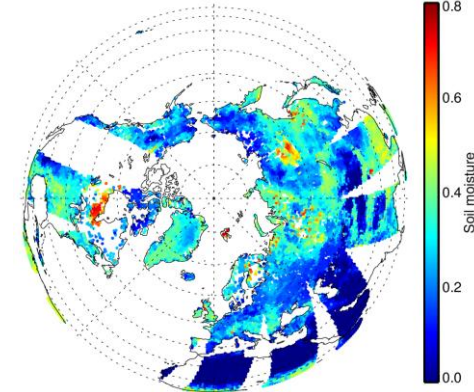
Labels



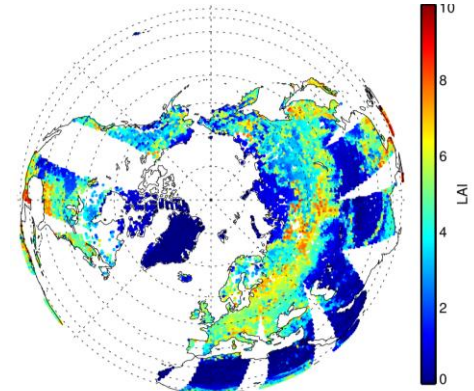
10 possible predictors for the brightness temperature

Skin temperature

Features



Soil moisture



Leaf area index

+ orography, snow depth, snow density, integrated water vapour, cloud, rain and snow water contents

Data preparation

Dataset of 470,000 observations and colocated model data

```
obdata = xr.open_dataset('/perm/rd/stg/odb/hkhg/ml_amsr2_chan9.nc')
```

```
x0 = np.column_stack([obdata.TSFC, obdata.SOIL_MOISTURE, obdata.SNOW_DEPTH, \
                    obdata.SNOW_DENSITY, obdata.LAI, obdata.OROGRAPHY, \
                    obdata.FG_TCWV, obdata.FG_CWP, obdata.FG_RWP, obdata.FG_IWP])
y0 = np.column_stack([obdata.OBSVALUE])
```

```
def x_normalise(x_orig):
    x_min = [200.0, 0, 0, 0, 0, 0, 0, 0, 0]
    x_max = [350.0, 0.75, 0.5, 300, 10, 5000, 70, 1, 2, 8]
    x_min = np.outer(np.ones(x_orig.shape[0]), np.array(x_min))
    x_max = np.outer(np.ones(x_orig.shape[0]), np.array(x_max))
    return (x_orig - (x_max+x_min)/2.0) / (x_max-x_min)*2.0
```

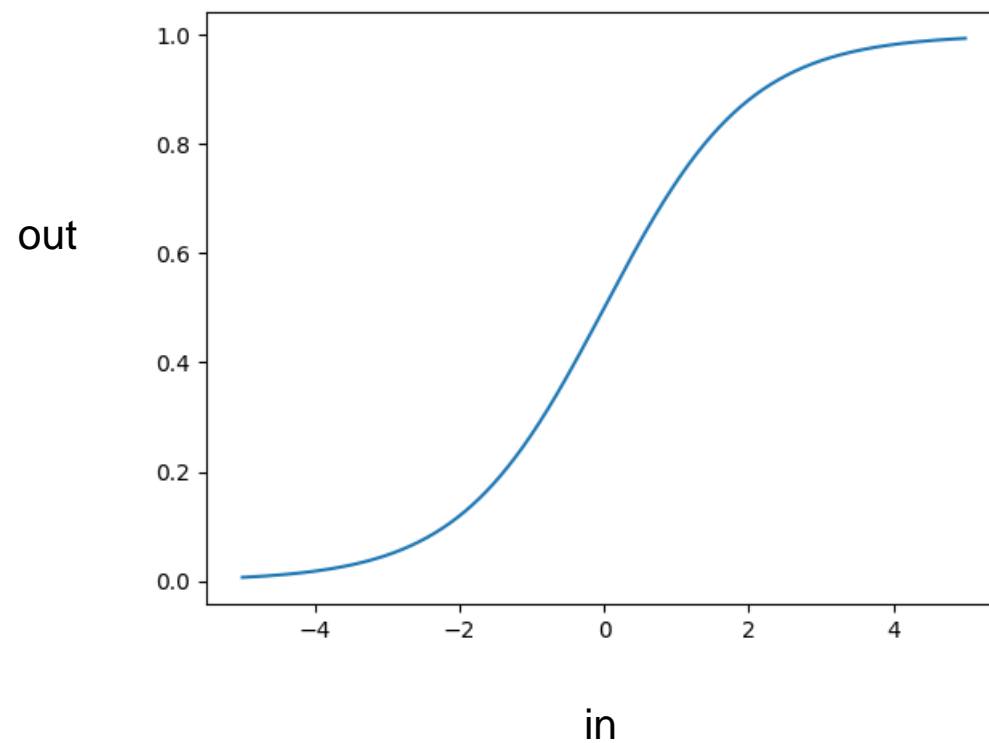
Prepare numpy arrays of correct shape for Keras

```
x1 = x_normalise(x0)
```

Normalise 'features' x to roughly -1 to +1

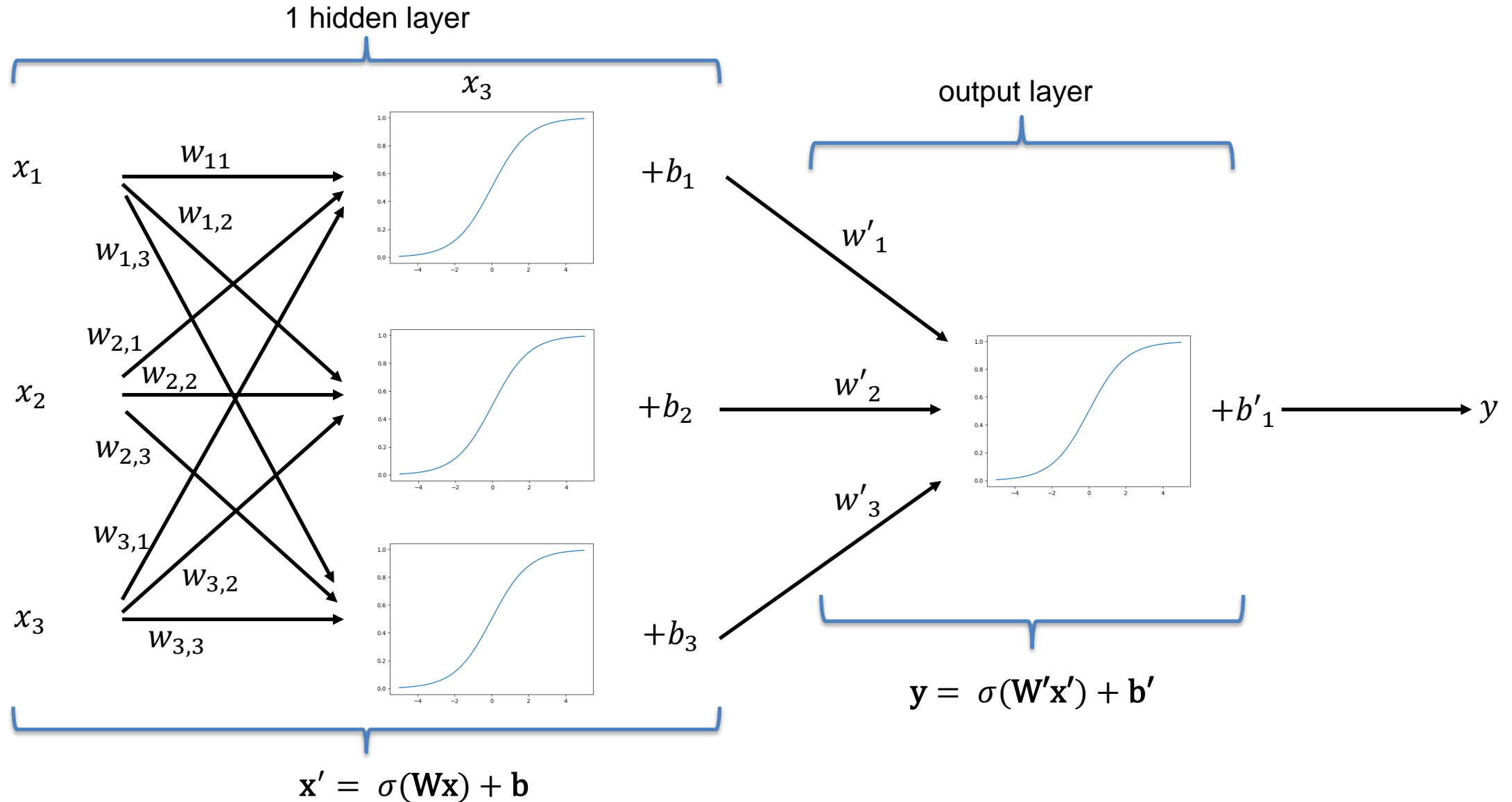
And... (not shown) normalise labels y to within 0 to 1

Sigmoid activation function $\sigma()$



```
b=np.arange(-5,5,0.01)  
plt.plot(b,1/(1+np.exp(-b)))
```


Feedforward neural network - example



Set up a neural network for the land surface observation operator

```
In [21]: model = Sequential()
...: model.add(Dense(units=10, activation='sigmoid', input_dim=10))
...: model.add(Dense(units=6, activation='sigmoid'))
...: model.add(Dense(units=1, activation='sigmoid'))
...: model.summary()
...:
...: model.compile(loss='mean_squared_error', optimizer='adam')
...:
```

Model: "sequential_2"

Layer (type)	Output Shape	Param #
dense_4 (Dense)	(None, 10)	110
dense_5 (Dense)	(None, 6)	66
dense_6 (Dense)	(None, 1)	7

Total params: 183
Trainable params: 183
Non-trainable params: 0

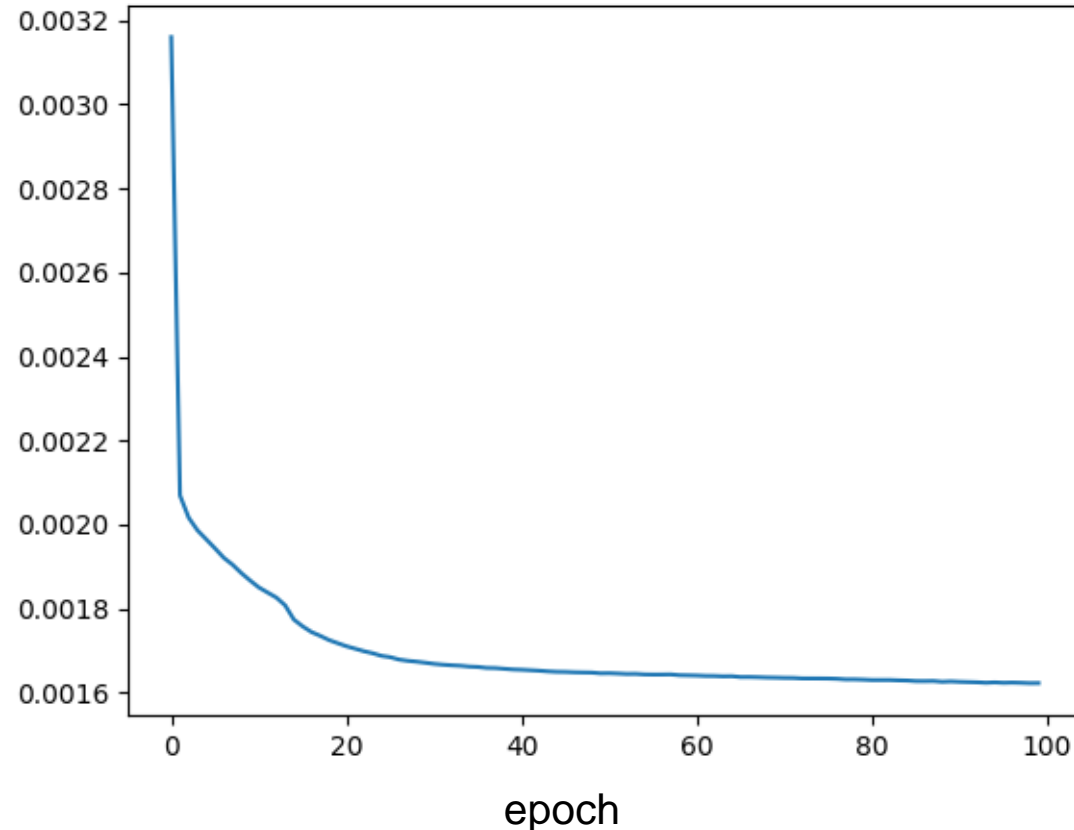
Train it (about 25 minutes on a linux workstation)

```
history = model.fit(x1, y1, epochs=100)
```

Loss function

$$J_{\text{obs}} = \frac{1}{n} \sum_{i=1}^n (y_{\text{obs},i} - y_{\text{sim},i})^2$$

Default “loss function” is just the 4D-Var J_0 without representation of observation error.



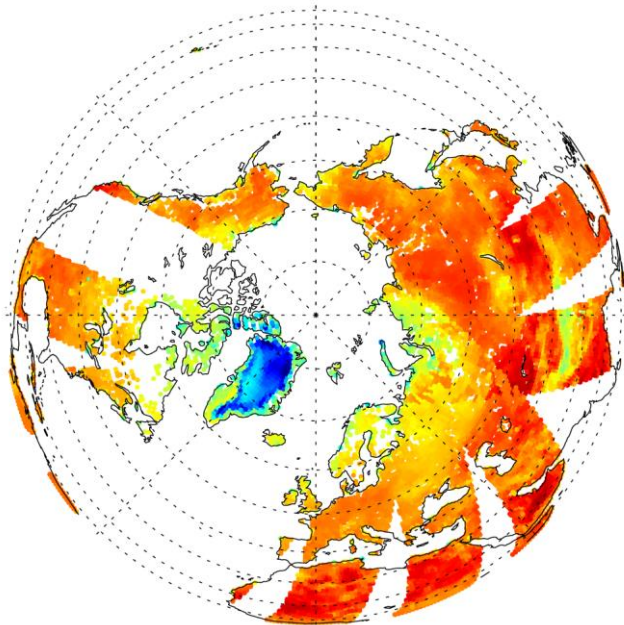
Adam – a sophisticated stochastic gradient descent (SGD) minimiser

“Backpropagation” is ML’s term for computing gradients of the cost function with respect to trainable parameters, using calls through the adjoints of each neural network layer.

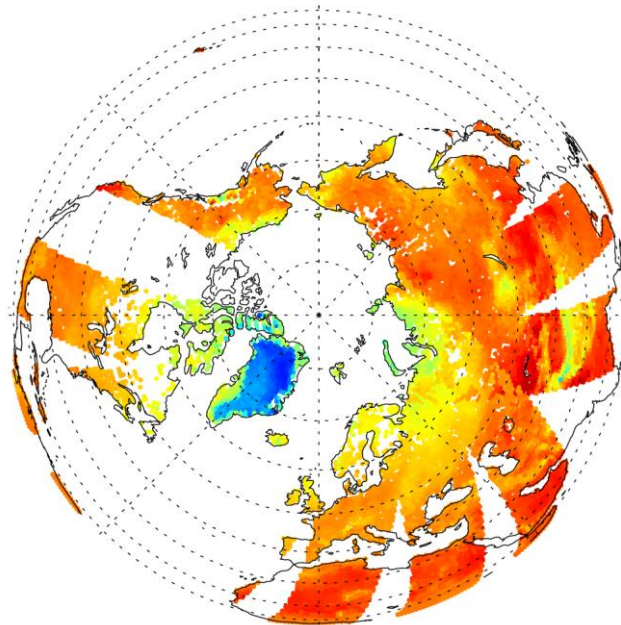
~Variational data assimilation without error representations, without regularisation, without state update

Results (ability to fit training dataset)

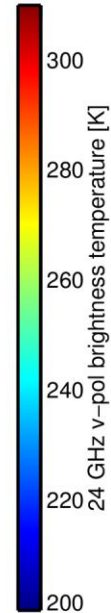
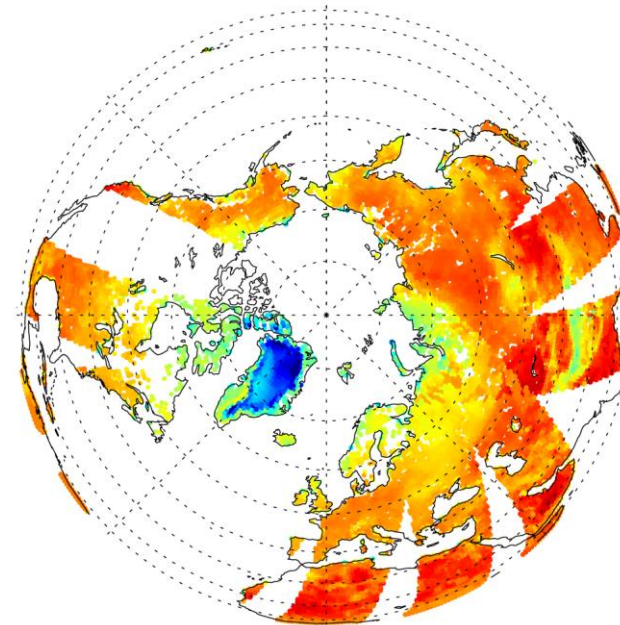
Observations



ML predicted



Physically-based simulation produced by IFS (RTTOV for atmosphere, dynamical emissivity retrieval for surface emissivity)



```
predict = y_unnormalise(model.predict(x1))
```



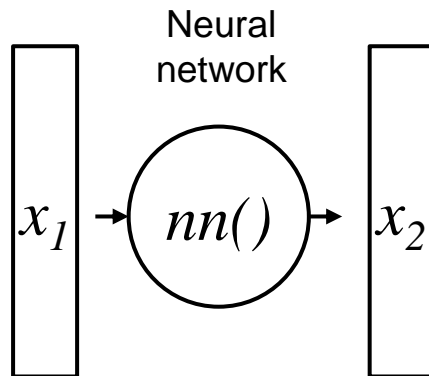
Hand-written function to recover TB

Problems with this toy NN model for 24 GHz radiances

- It's not as good as the current physical methods
- The input variables are not sufficient to drive the outputs
 - Missing variables – e.g. over Greenland, detailed knowledge of snow and ice microstructure
- One of the driving problems for all-surface data assimilation:
 - Neither the models nor the input state are fully known
 - Chicken and egg problem: can't train the model if you don't know the necessary inputs well enough

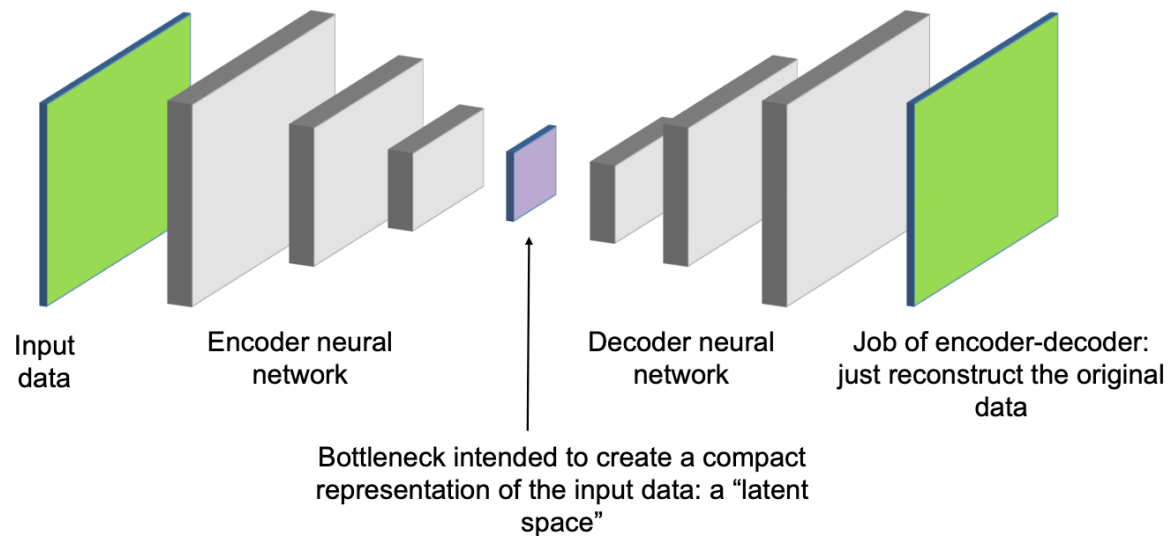
Types of ML

Types of ML – supervised learning



Supervised learning:

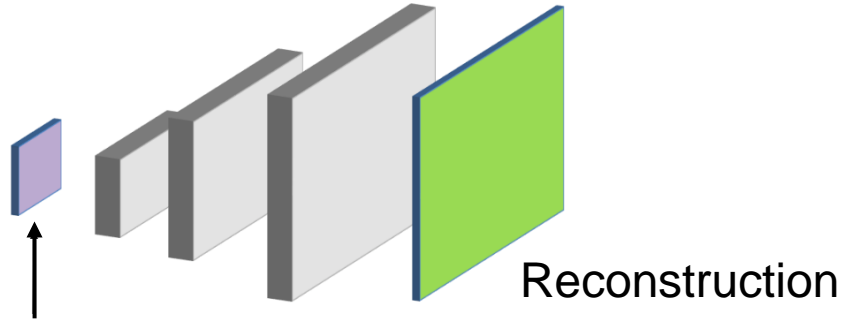
- ML as a "universal function approximator" (Hornik, 1991)
- Both inputs x_1 and outputs x_2 need to be provided as training data
- An "emulator" / "surrogate" / "empirical model"



Encoder-decoder:

- Data compression
- Data assimilation in the space of an autoencoder (Peyron et al., 2021)
- Still needs both inputs and outputs to train the model

Types of ML – unsupervised learning – generative ML

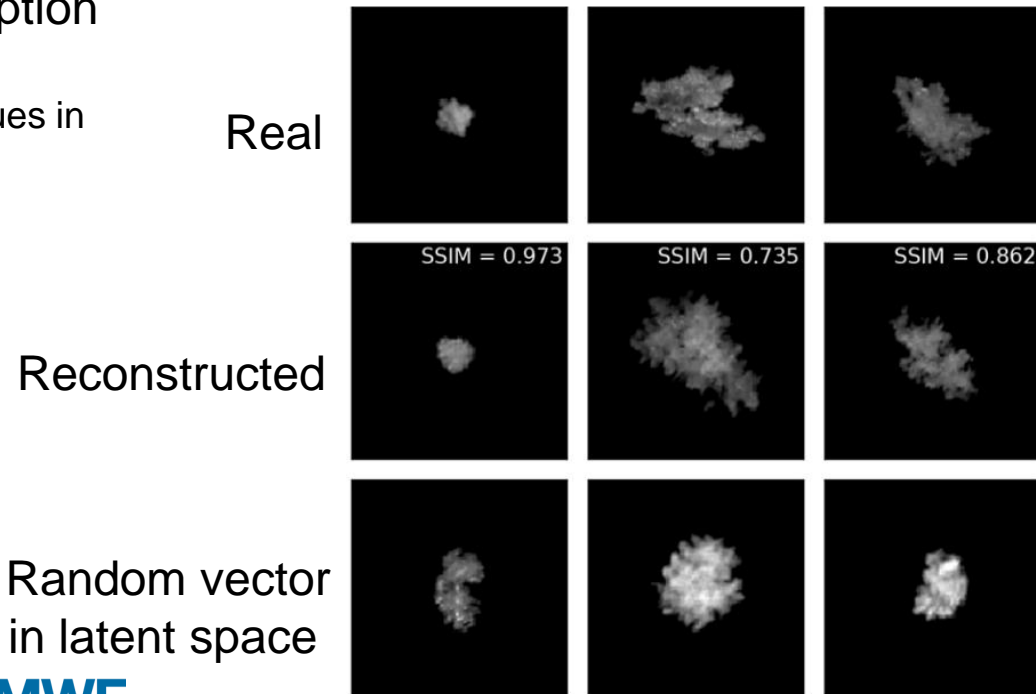


Latent space: a reduced statistical description of a phenomenon

A bit like a set of eigenvalues in a principal component decomposition

What if we could just have the decoder?

- How do we train it?
 - We could train an encoder-decoder on something, and then throw away the encoder.
 - Or find some more clever way...



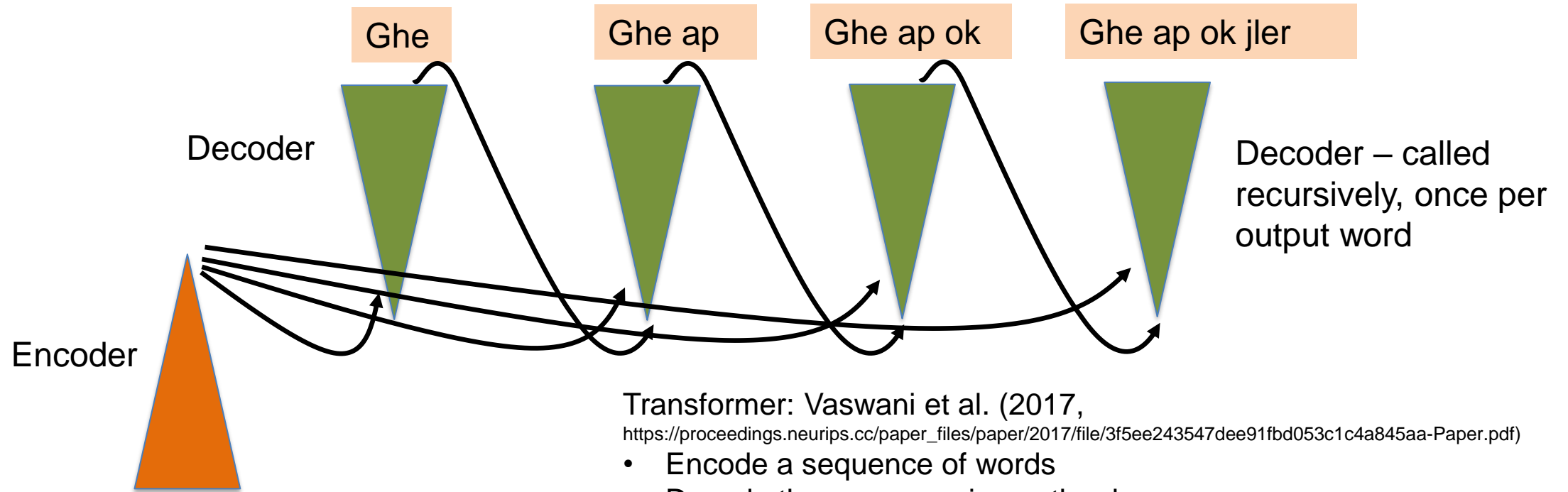
Snowflake images from Leinonen and Berne (2021, <https://doi.org/10.5194/amt-13-2949-2020>)

Generative Adversarial Network (GAN):

- Generator (~decoder): make an image
- Discriminator (~encoder): given an image, tell if it is real or fake -> drives the loss function

Generative ML - transformers

Outputs – translate to another language (original google application) – or continue in same language (GPT-1)



Thg hrt de pyur otr gasfas nff a bgu

Inputs – in one language (whole word sequence at once)

Transformer: Vaswani et al. (2017, https://proceedings.neurips.cc/paper_files/paper/2017/file/3f5ee243547dee91fbd053c1c4a845aa-Paper.pdf)

- Encode a sequence of words
- Decode the sequence in another language
- "attention mechanism", "positional encoding" etc..

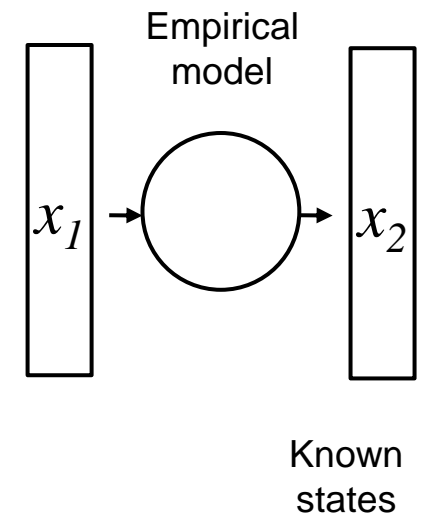
Generative Pre-trained Transformer (GPT)

- GPT-1 is *just* a transformer like this (120 million parameters)
- GPT-2/3/4 architecture is not public but broadly an extension of these concepts (parameters: v3: 175 billion, v4: 1000 billion???)

How ML can benefit DA

What does ML bring for data assimilation? 1) surrogate modelling

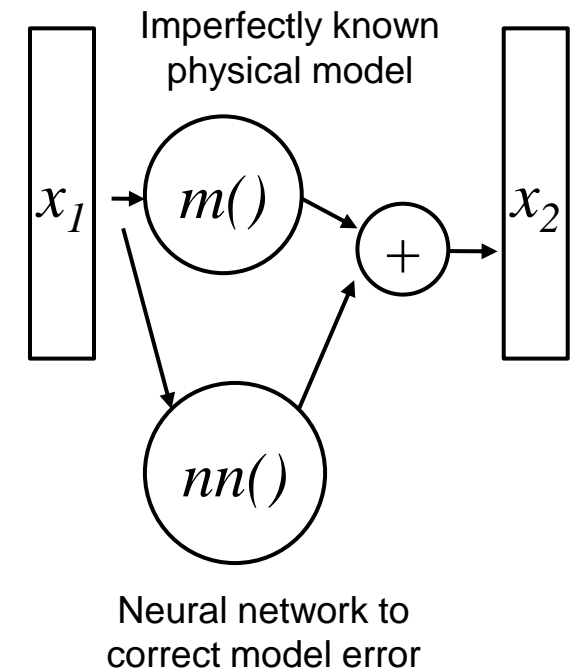
- Train against existing datasets, typically an existing physical model
- Acceleration:
 - E.g. use many more ensemble members, allowing previously unaffordable data assimilation algorithms (Chattopadhyay et al. , 2021, GMDD, <https://doi.org/10.5194/gmd-2021-71>, generate a 1000-member ensemble)
 - E.g. generate samples of model error from which to derive a model error covariance matrix: Bonavita and Laloyaux, 2022 (<https://arxiv.org/abs/2209.11510>)
- Space compression:
 - E.g. data assimilation in the latent space of an auto encoder (Peyron et al., 2021, Latent space data assimilation by using deep learning <https://arxiv.org/abs/2104.00430>)
- Numerical differentiation:
 - E.g. provide a tangent linear and adjoint for variational data assimilation: Gravity wave drag scheme emulated by ML and then ML used to provide TL/adjoint: Hatfield, Chantry et al., 2021(<https://doi.org/10.1029/2021MS002521>)



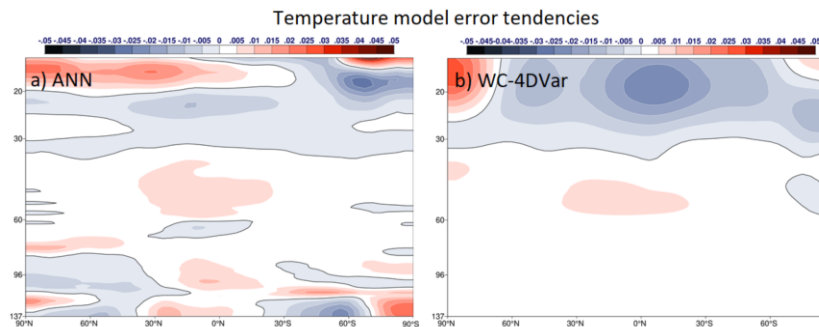
What does ML bring for data assimilation? 2) bias correction

Correct model or observation error:

- Train against historical data assimilation increments or departures
- Or train “online” inside a data assimilation system
 - Separate, iterative approach (e.g. Brajard et al., 2020, <https://doi.org/10.1016/j.jocs.2020.101171>)
 - Online training inside variational data assimilation is in development
- A nonlinear extension to existing data assimilation bias correction methods
 - Weak constraint data assimilation
 - Parameter estimation
 - Variational bias correction (VarBC)
- Example: model error correction in IFS, Bonavita and Laloyaux, 2020 (<https://doi.org/10.1029/2020MS002232>)



Neural network estimate of model bias



Weak constraint 4D-Var

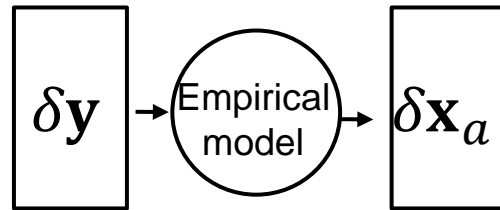
What does ML bring for data assimilation? 3) replace entire DA system

The analysis equation

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}(\mathbf{y} - H\mathbf{x}_b)$$

(model space)

$$\delta\mathbf{x}_a = \mathbf{K}\delta\mathbf{y} \quad (\text{observation space})$$



\mathbf{x}_a - analysis vector
 \mathbf{x}_b - background vector
 \mathbf{y} - observation vector
 $H(\mathbf{x}_b)$ - forward observation operator
 \mathbf{H} - Jacobian or tangent linear approximation of H
 \mathbf{R} - observation error covariance
 \mathbf{B} - background error covariance
 $\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}$ Kalman gain matrix
 $\delta\mathbf{y} = \mathbf{y} - H\mathbf{x}_b$ is the innovation vector
 $\delta\mathbf{x}_a = \mathbf{x}_a - \mathbf{x}_b$ is the analysis increment

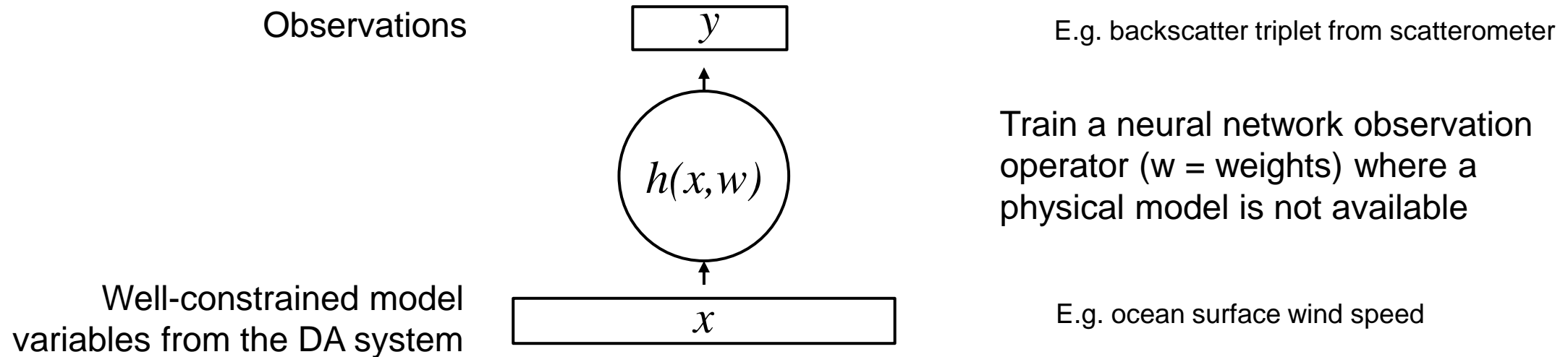
- Train an ML model to do the DA step – e.g. take innovations $\delta\mathbf{y}$ and produce increments $\delta\mathbf{x}_a$
 - Cintra et al. (2016, Tracking the model: Data assimilation by artificial neural network. In *2016 International Joint Conference on Neural Networks (IJCNN)* (pp. 403-410))
 - Arcucci et al. (2021, <https://doi.org/10.3390/app11031114>)
- Problems:
 - Most work so far has been done on simple test systems (e.g. Lorenz '63)
 - Real DA uses $H()$ operator to map diversely in space, time and to observable variables (e.g. observation space)
 - How do we adapt to new observation types? How much training (and retraining) is needed?

What does ML bring for data assimilation? 4) learn new models

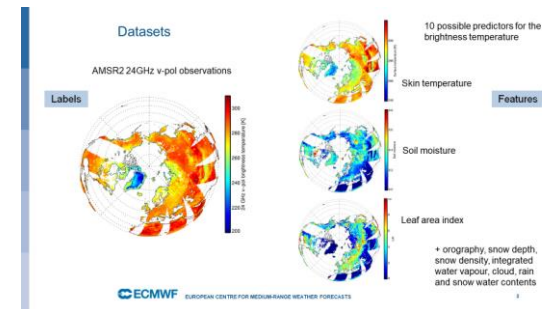
Learn new models directly from observations, where physical models do not exist or are not good enough:

- If we train an ML forecasting model against analysis, it learns to map analyses (the combination of forecast and observations) not forecast state to forecast state (if training to a physical forecast model)
 - ML forecasting models like Pangu-Weather or Graphcast may already be encoding some “new physics” – at minimum, online bias corrections
- Train against high resolution models (e.g. train moist physics scheme for a GCM against a convection resolving model)
- Train directly against observations?
 - Irregular and indirect link to observation space makes this hard
 - Solution? **Train empirical components inside a physical DA system**

What does ML bring for data assimilation? 5) new observation operators



- Example: land surface radiances at microwave frequencies



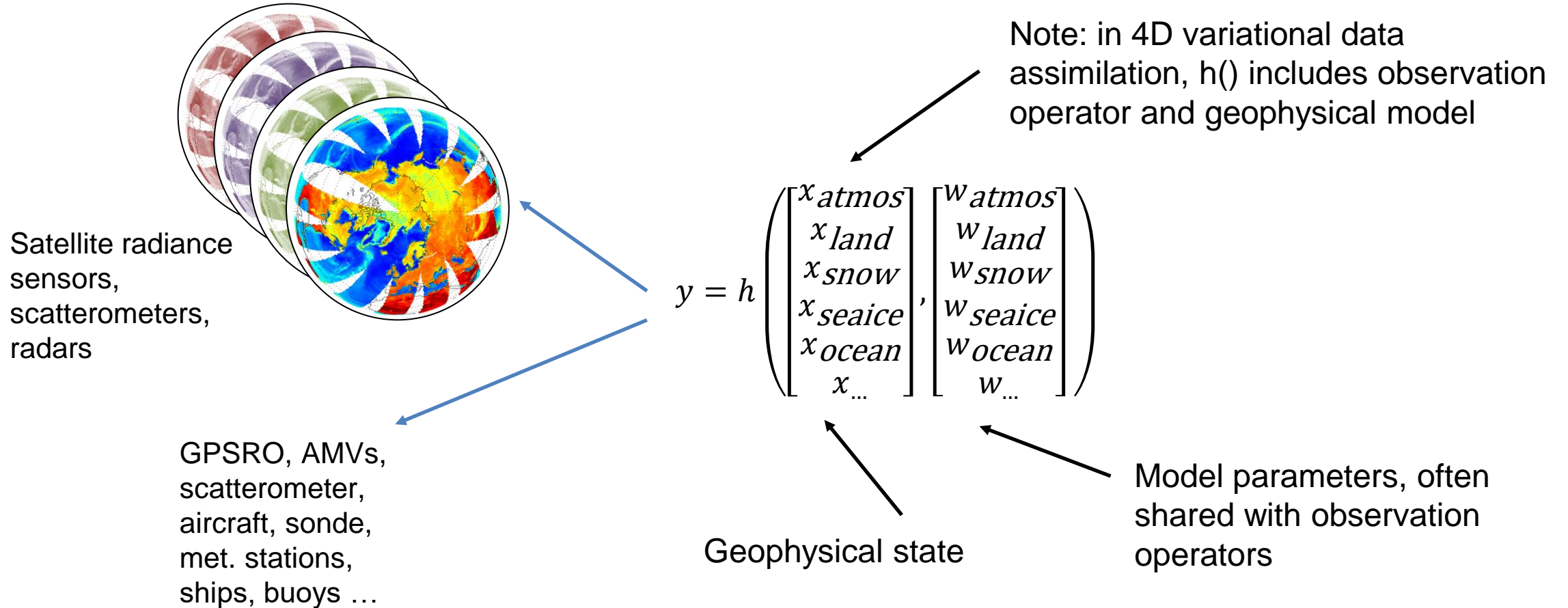
- Example (in retrieval direction) operationally used at ECMWF for soil moisture assimilation from SMOS: Rodriguez-Fernandez et al., 2019, "SMOS Neural Network Soil Moisture Data Assimilation in a Land Surface Model and Atmospheric Impact", <https://www.mdpi.com/2072-4292/11/11/1334>

Theoretical links between ML and DA

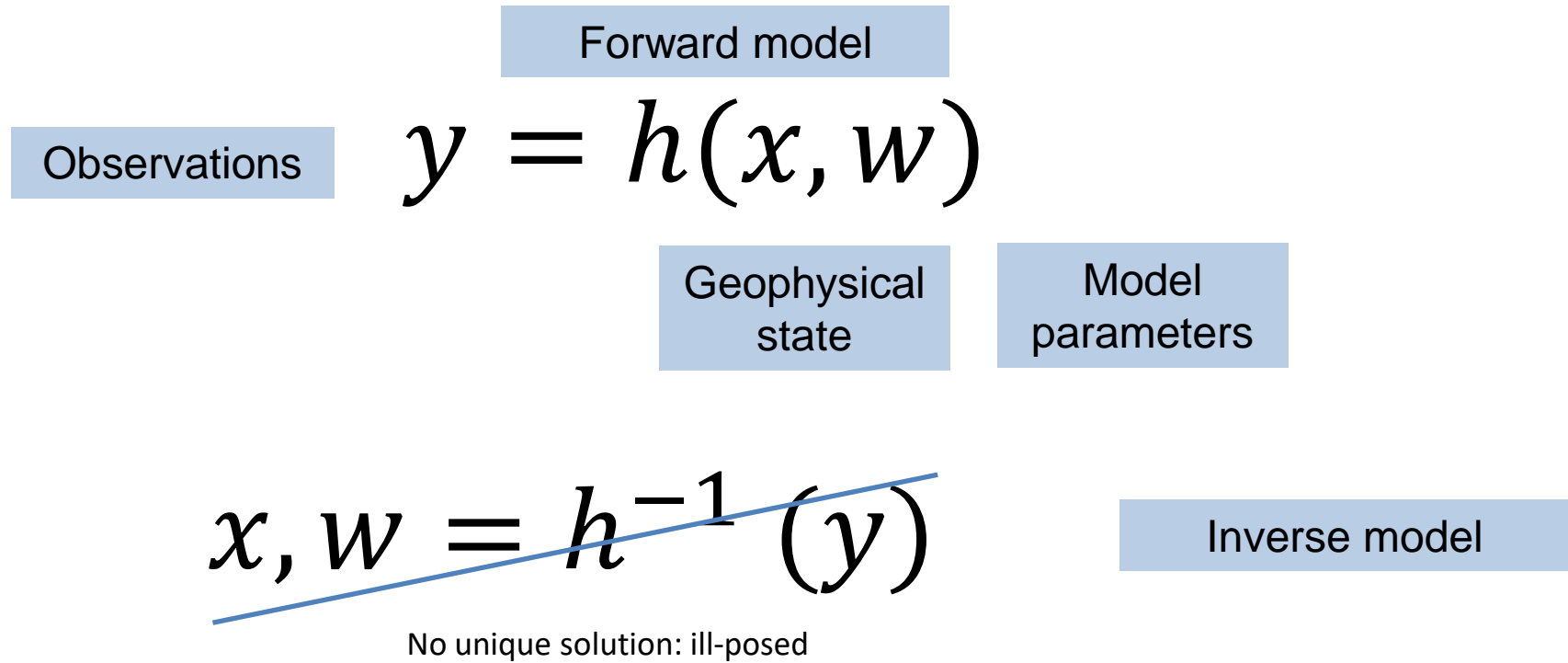
4D coupled earth system assimilation

Observations

Forward model: observation operator and geophysical models

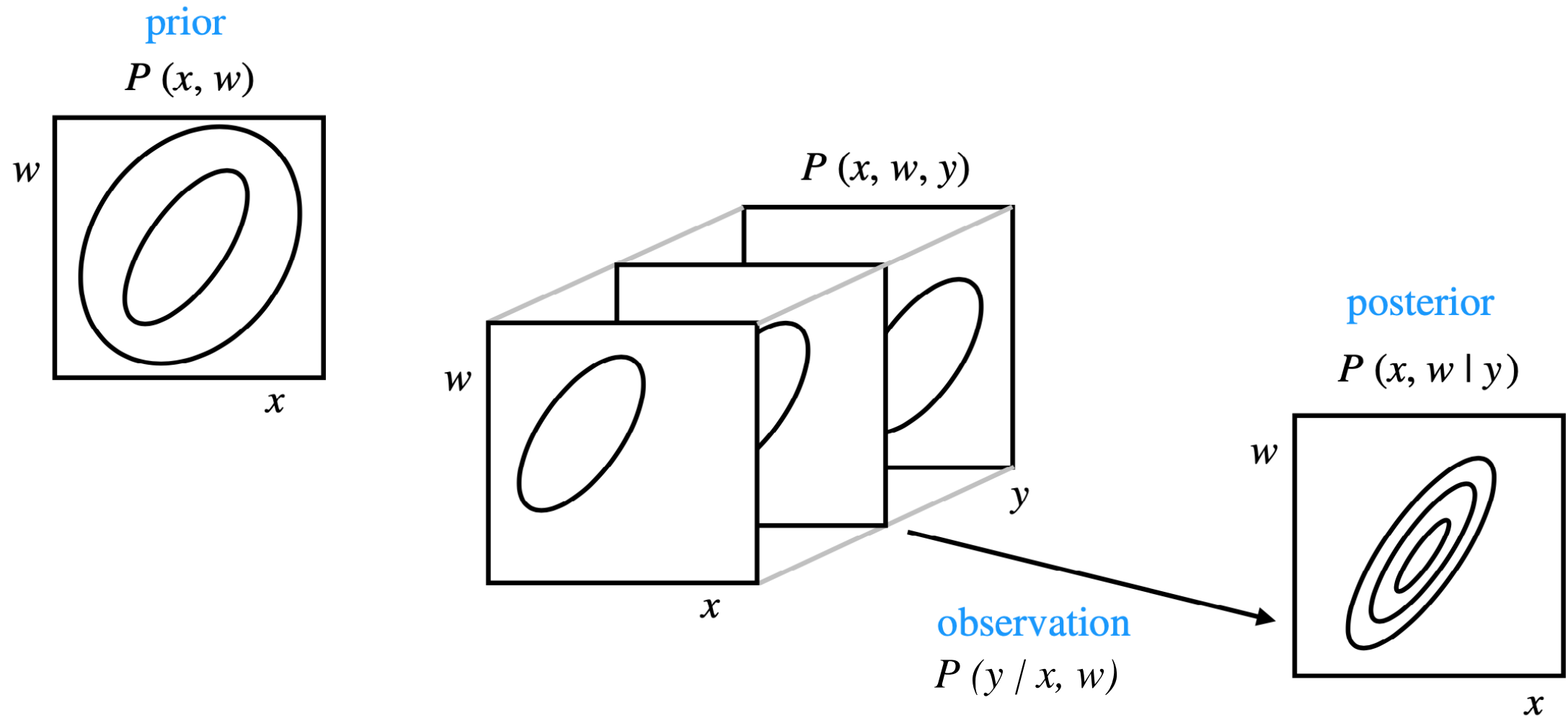


The forward and inverse problem



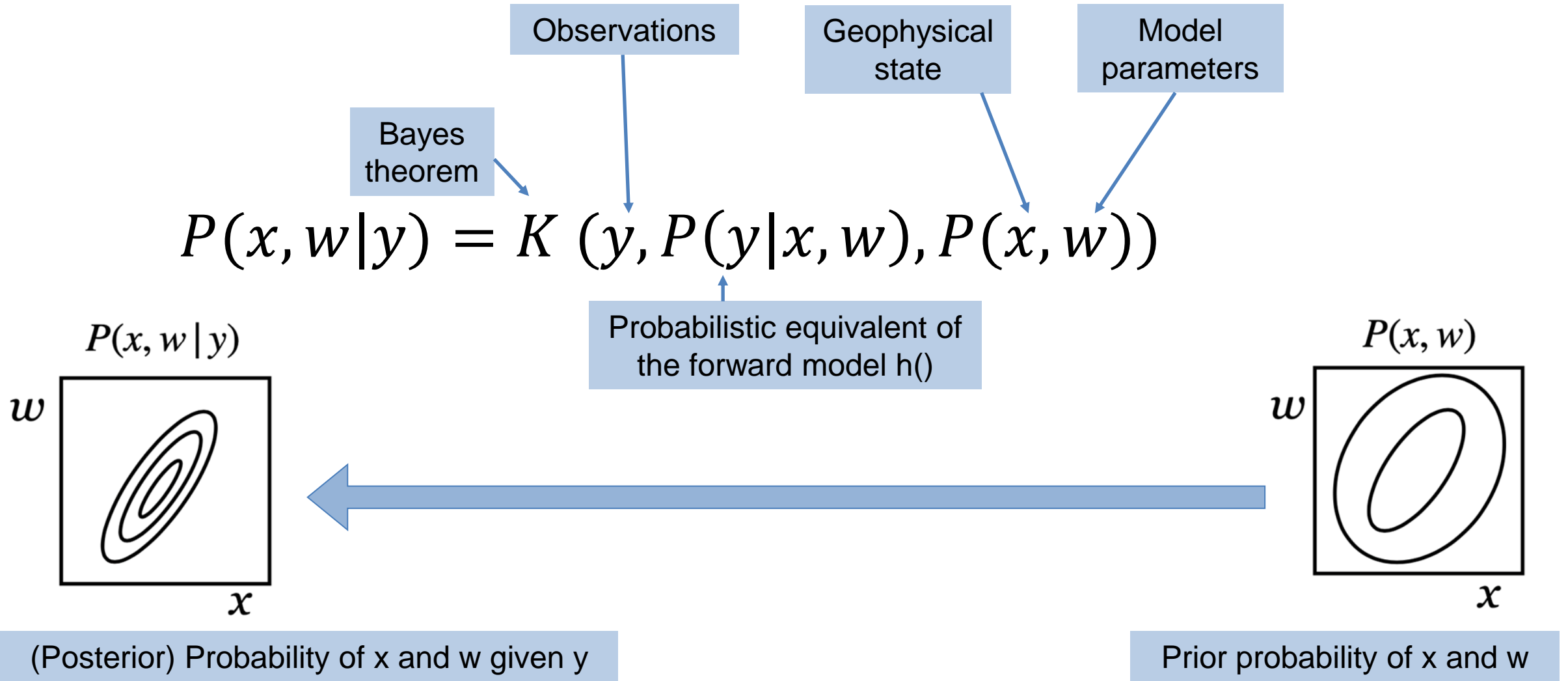
The best that observations can do is to provide a statistical improvement in our knowledge of x and w

Bayes' theorem



The inverse problem solved by Bayes theorem

as the first lecture of this DA course, but extended with state AND parameters



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

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

A diagram with the text "Prior (background)" at the top. Two arrows point downwards from this text to the terms Jx and Jw in the equation above. Jx is associated with "Prior knowledge of state" and Jw is associated with "Prior knowledge of model".

DA Cost function

Observation term

Prior knowledge of state

Prior knowledge of model

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

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

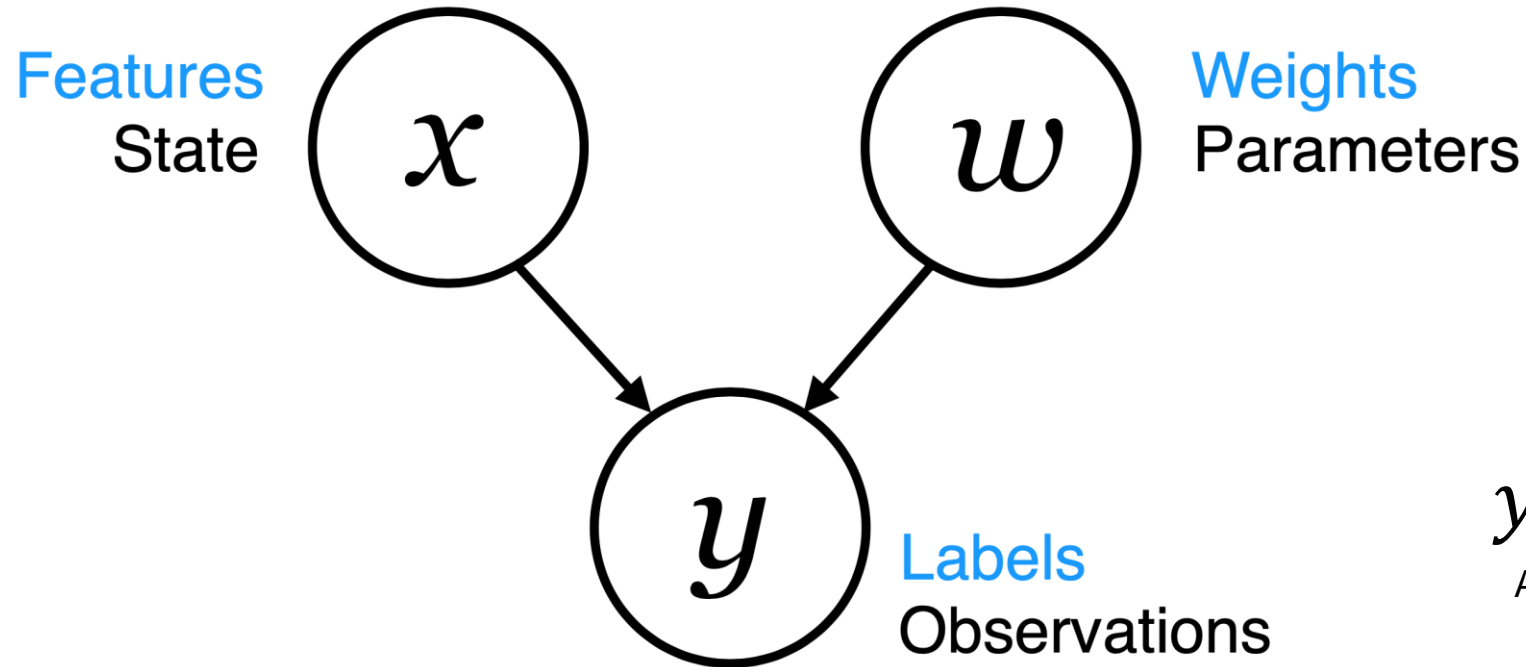
Machine learning (e.g. NN)

Variational data assimilation

Labels	y	Observations	y^o
Features	x	State	x
Neural network or other learned models	$y' = W(x)$	Physical forward model	$y = H(x)$
Objective or loss function	$(y - y')^2$	Cost function	$J = J^b + (y^o - H(x))^T R^{-1} (y^o - H(x))$
Regularisation	$\ w\ $	Background term	$J^b = (x - x^b)^T B^{-1} (x - x^b)$
Iterative gradient descent		Conjugate gradient method (e.g.)	
Back propagation		Adjoint model	$\frac{\partial J}{\partial x} = H^T \frac{\partial J}{\partial y}$
Train model and then apply it		Optimise state in an update-forecast cycle	

Boukabara et al. (2021) <https://doi.org/10.1175/BAMS-D-20-0031.1>

Bayesian equivalence of ML and DA

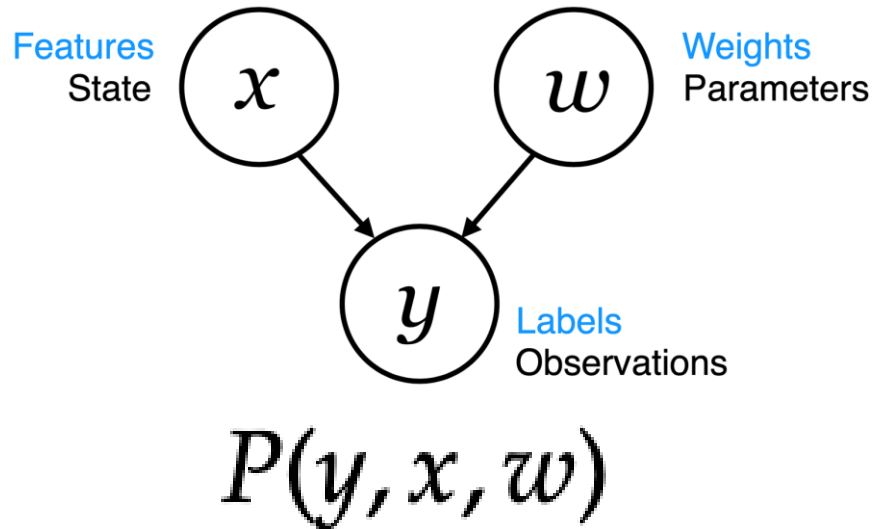


$$y = h(x, w)$$

As a Bayesian network

- Geer (2021)** <https://doi.org/10.1098/rsta.2020.0089>
- 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](https://doi.org/10.1175/1520-0477(1998)079%3C1855:ANNMTP%3E2.0.CO;2)
- Goodfellow et al. (2016) <https://www.deeplearningbook.org>

Bayesian networks: representing the factorisation of joint probability distributions



1. Factorise in two different ways using the chain rule of probability

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

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

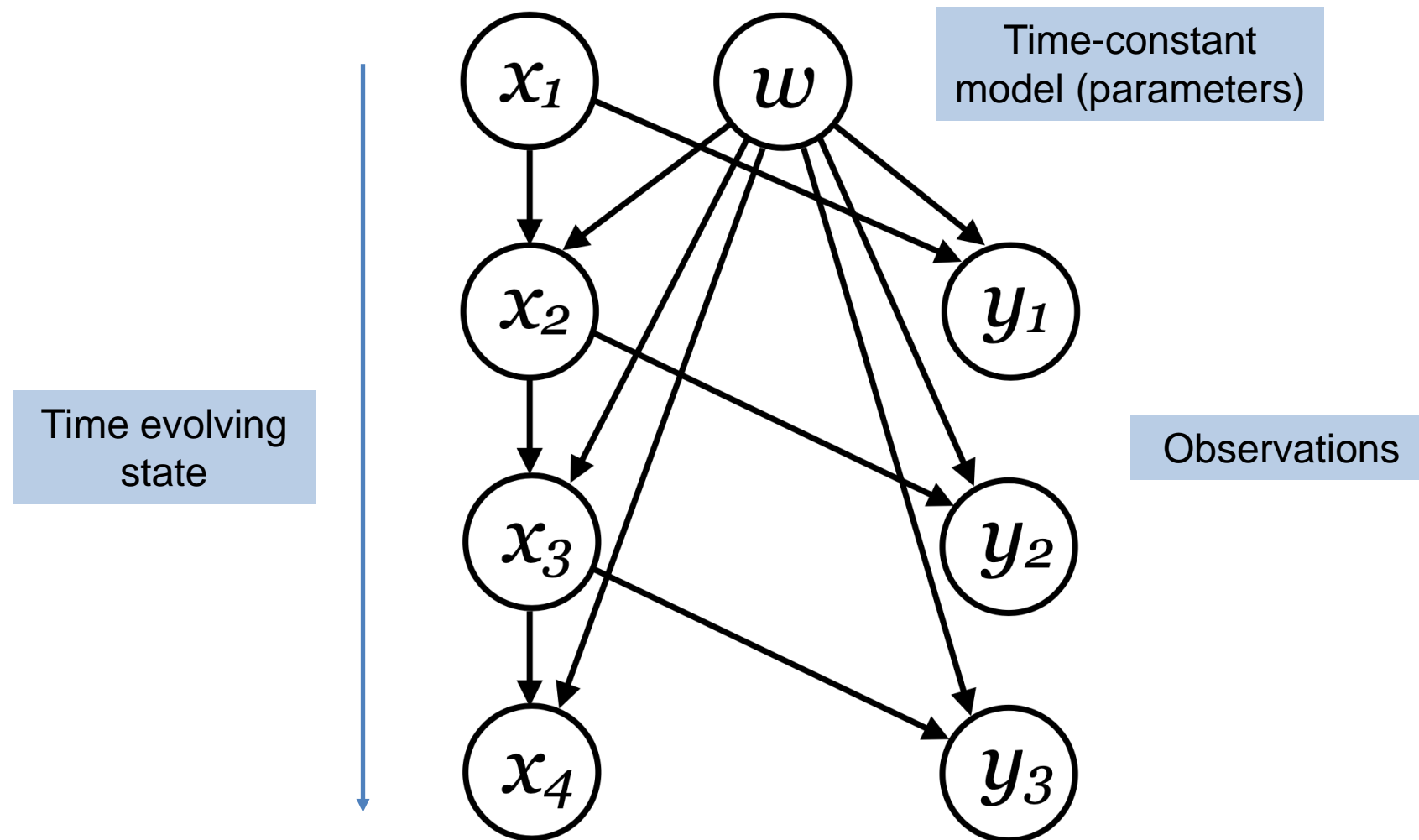
2. Equate the two right hand sides and rewrite

$$P(x|w, y)P(w|y) = \frac{P(y|x, w)P(x|w)P(w)}{P(y)}$$

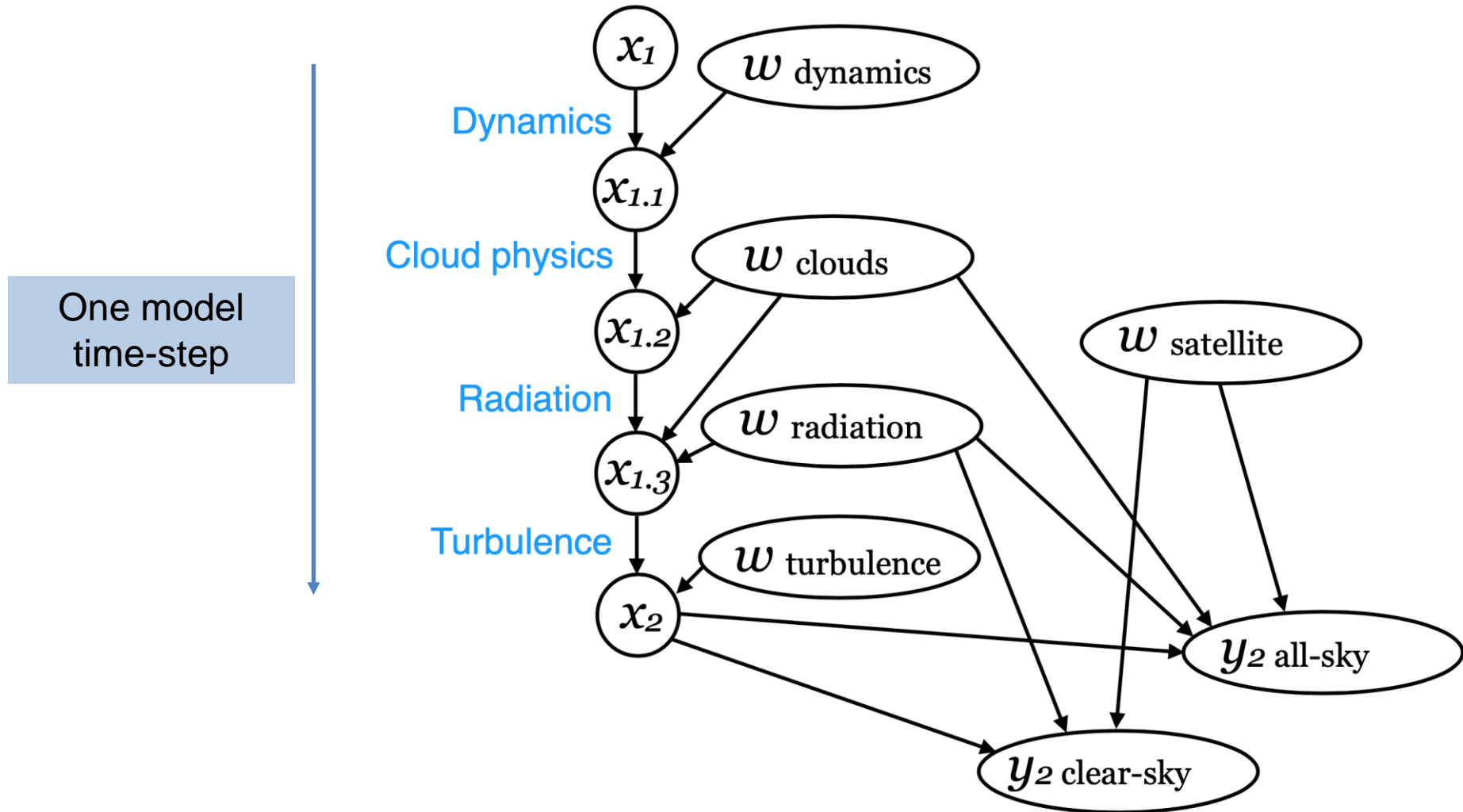
3. Rewrite by putting back the joint distributions of x,w: Bayes' rule

$$P(x, w|y) = \frac{P(y|x, w)P(x, w)}{P(y)}$$

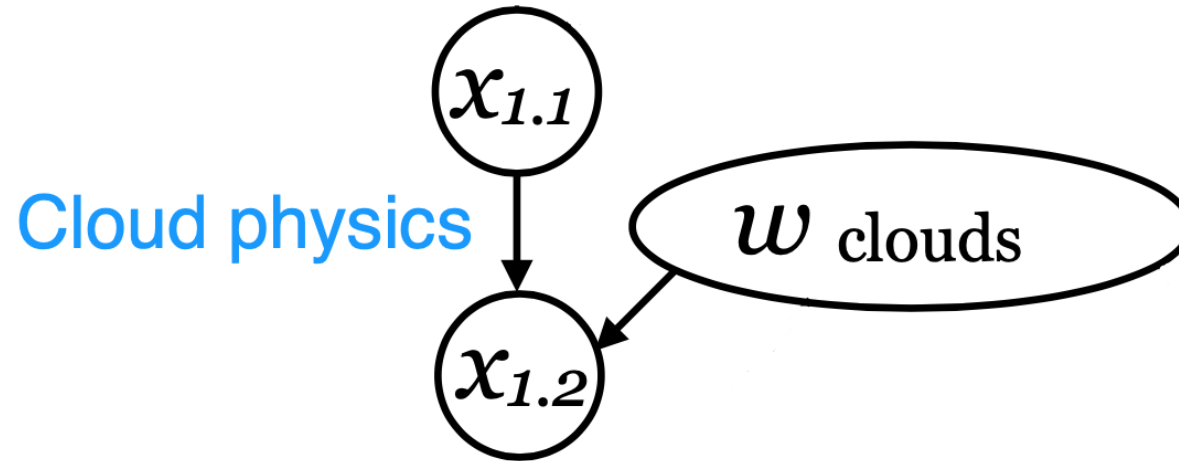
Time evolution of state – cycled data assimilation



Inside an atmospheric model & data assimilation timestep

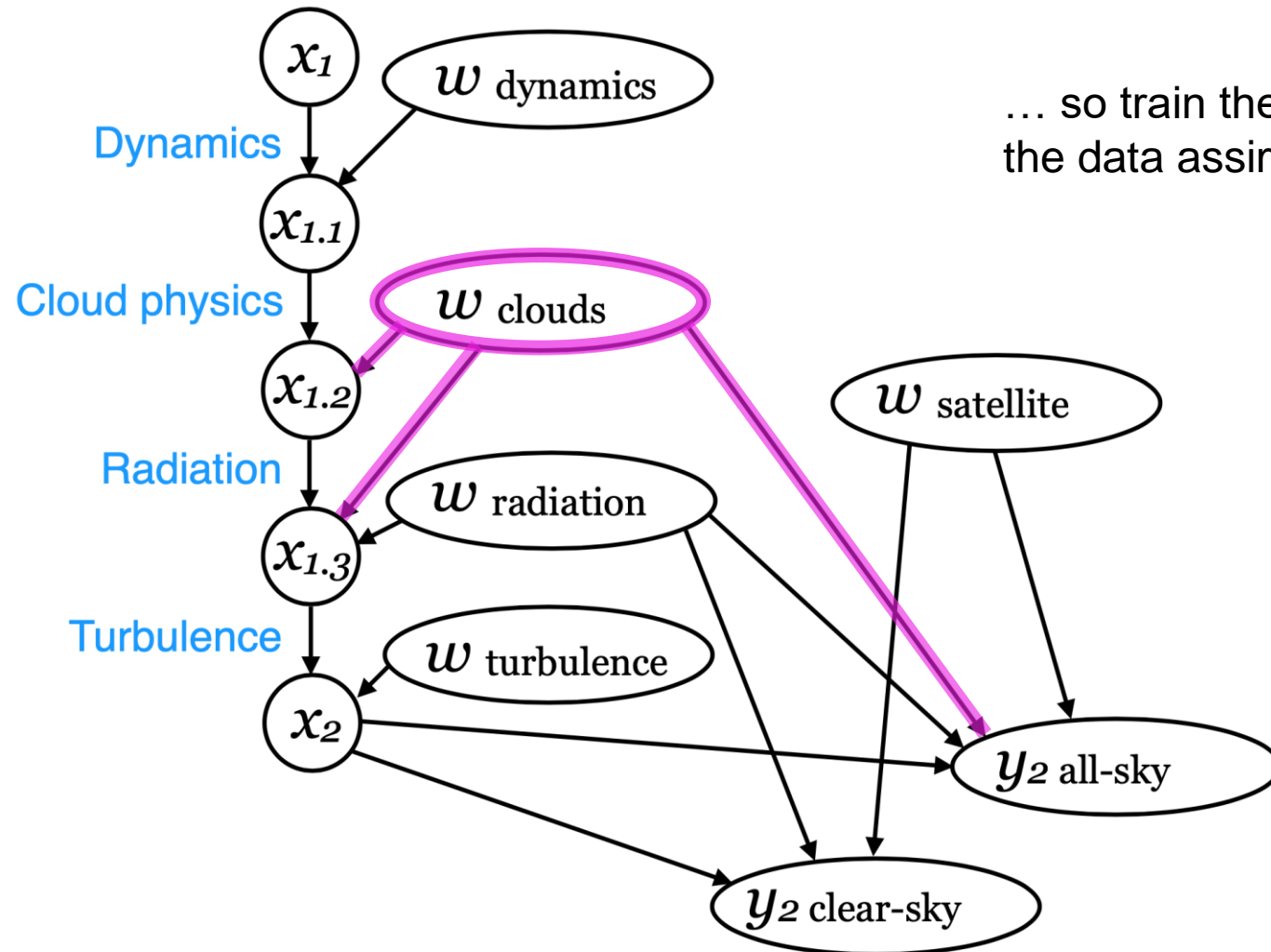


Learning an improved model of cloud physics (ML or DA)



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



Current issues and ideas combining machine learning and DA / physics

A few highlights from a rapidly developing new field

Combine physical and empirical models: Physically constrained ML

```
def net_u(self, x, t):  
    u = self.neural_net(tf.concat([x,t],1), self.weights, self.biases)  
    return u
```

Neural network

```
def net_f(self, x,t):  
    u = self.net_u(x,t)  
    u_t = tf.gradients(u, t)[0]  
    u_x = tf.gradients(u, x)[0]  
    u_xx = tf.gradients(u_x, x)[0]  
    f = u_t + u*u_x - self.nu*u_xx  
  
    return f
```

Gradients of the network

Burger's equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0$$

```
self.loss = tf.reduce_mean(tf.square(self.u_tf - self.u_pred)) + \  
            tf.reduce_mean(tf.square(self.f_pred))
```

Custom loss function

<https://github.com/maziarraissi/PINNs>

Raissi, Maziar, Paris Perdikaris, and George Em Karniadakis. "[Physics Informed Deep Learning \(Part I\): Data-driven Solutions of Nonlinear Partial Differential Equations.](#)" [arXiv preprint arXiv:1711.10561 \(2017\)](#)

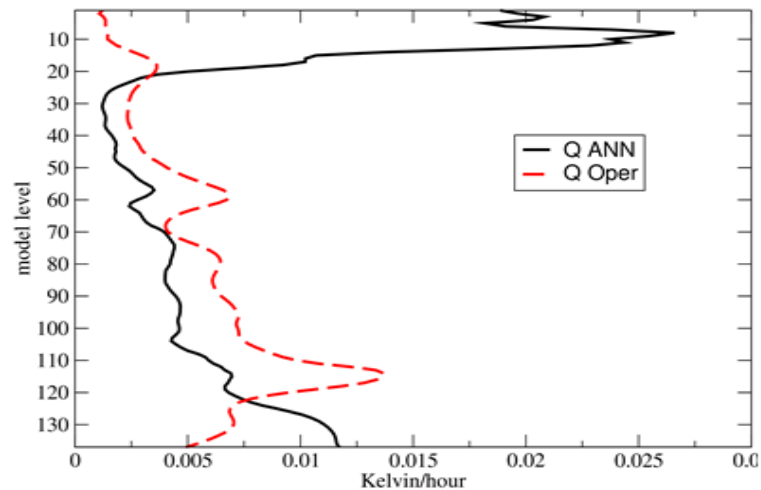
Hybrid data assimilation and machine learning: train the neural network (forecast model, or bias correction) as part of the data assimilation process

- Simultaneous estimation of the initial conditions, NN parameters and dynamical parameters of a model (e.g. Lorenz '63) using data assimilation (Hsieh and Tang, 2001, [https://doi.org/10.1175/1520-0493\(2001\)129<0818:CNNTID>2.0.CO;2](https://doi.org/10.1175/1520-0493(2001)129<0818:CNNTID>2.0.CO;2))
- Use iterative cycles of data assimilation followed by neural network training (Brajard et al., 2020, <https://doi.org/10.1016/j.jocs.2020.101171>)
- In development at ECMWF – train a NN **within 4D-Var** – quasi-geostrophic (QG) model / OOPS
 - “Online model error correction with neural networks in the incremental 4D-Var framework”
 - Alban Farchi, Marcin Chrust, Marc Bocquet, Patrick Laloyaux, Massimo Bonavita (2022, <https://doi.org/10.48550/arXiv.2210.13817>)
- “Online learning” or sequential learning is a thing in ML too (compared to “train once” approach)
 - 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>

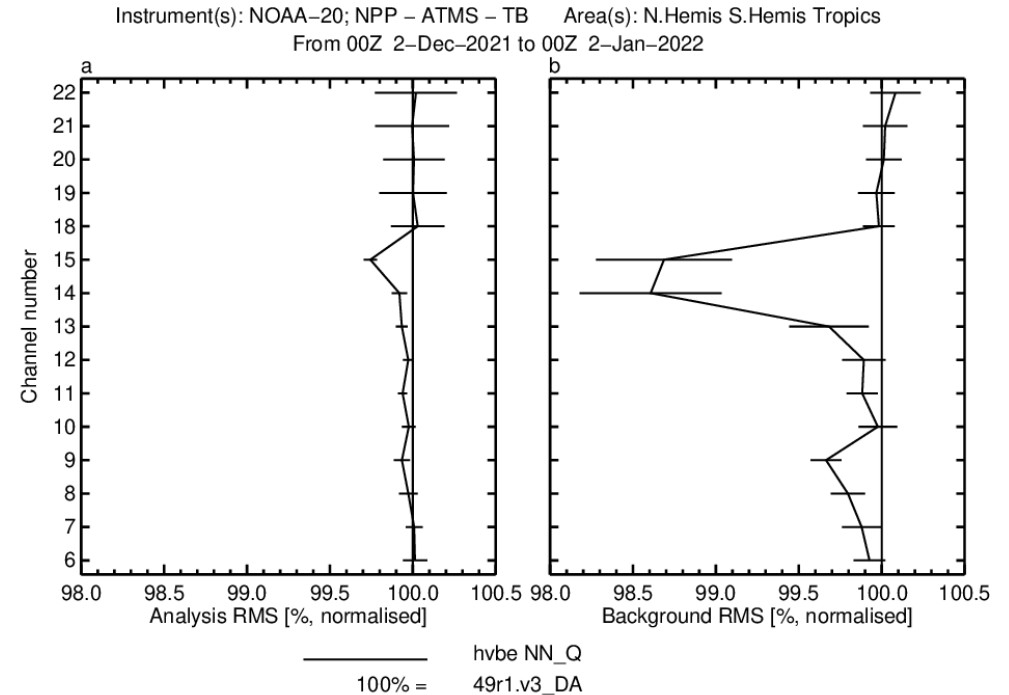
Online bias correction / weak-constraint 4D-Var

Massimo Bonavita, Patrick Laloyaux

- Evolution of WC-4Dvar: **NN-derived Q** matrix (equivalent of B matrix, but for weak constraint model error correction) and extension to **lower stratosphere (200 hPa)**
- Early version documented in <https://doi.org/10.48550/arXiv.2209.11510>



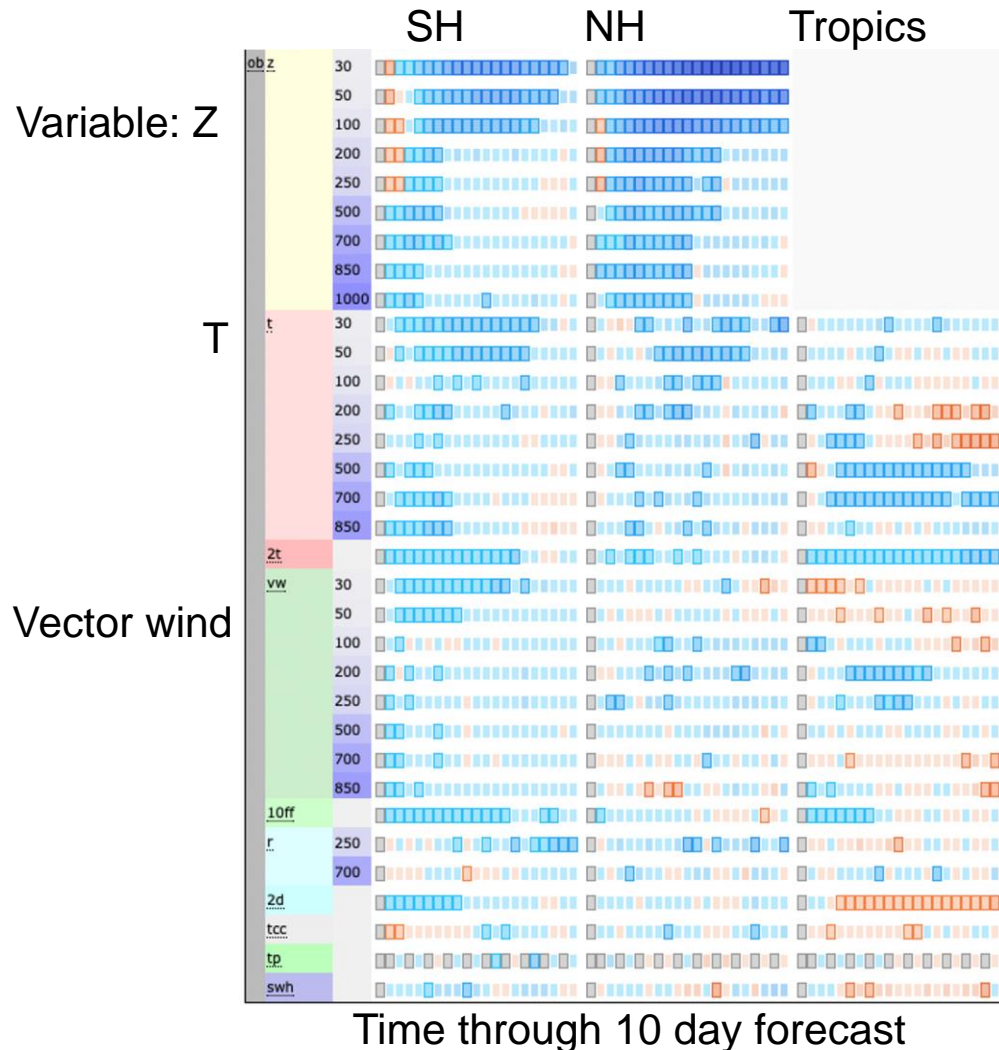
Example Q matrices



Improved fit to stratospheric temperature sounding channels at analysis and background (due to model T bias reduced)

The real payoff: apply online model bias corrections in the forecast model

Marcin Chrust, Alban Farchi, Patrick Laloyaux, Massimo Bonavita



**Score cards
(verifications against
observation, 3 DEC
2020 – 28 FEB 2021)**

Exp: Online NN model
error correction (1-
hourly) applied in
FCLONG (1-hourly) with
reduced magnitude:

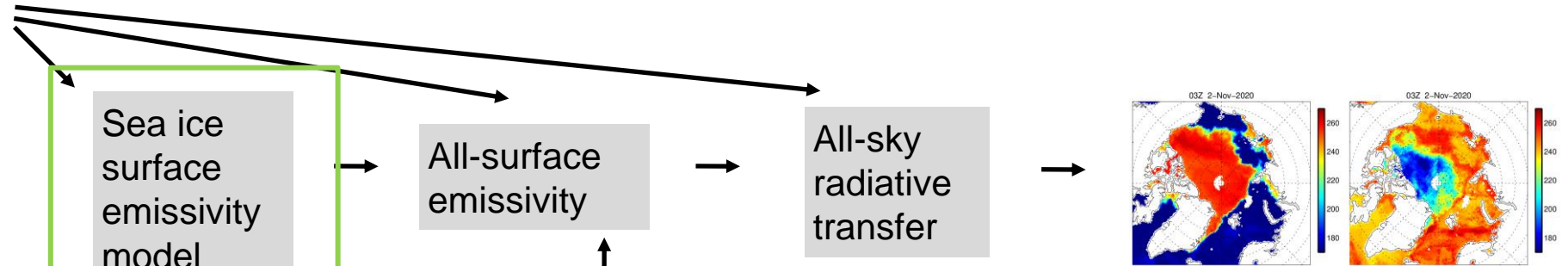
Control has no online
model error correction

Blue = reduced forecast error in experiment compared to
control (red = increased)

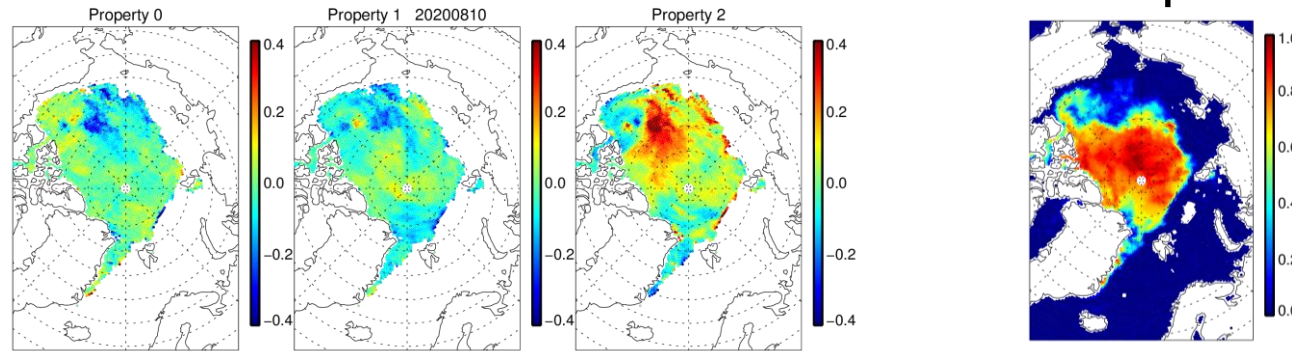
Learn a sea ice surface emissivity model using hybrid ML-DA techniques

Geer (2023) in preparation or come to ISDA online, 2nd June - <https://isda-online.univie.ac.at>

Inputs from IFS at 64 million observation locations:
background atmosphere and surface - Radiative transfer terms from RTTOV-SCATT, effective cloud fraction, skin temperature, ocean surface emissivity, location etc.



1 year of AMSR2 radiance observations at 64 million locations for 10 channels (10 – 89 GHz, v/h)



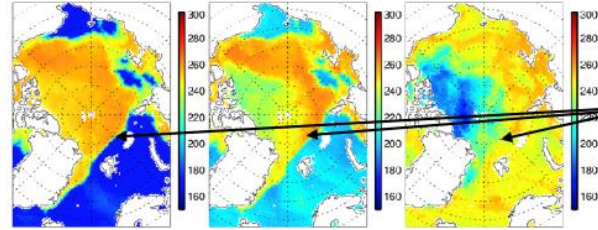
Gridded empirical surface emissivity properties
62000 points on 40 km grid
365 days
3 surface properties

Gridded sea ice fraction
62000 points on 40 km grid
365 days

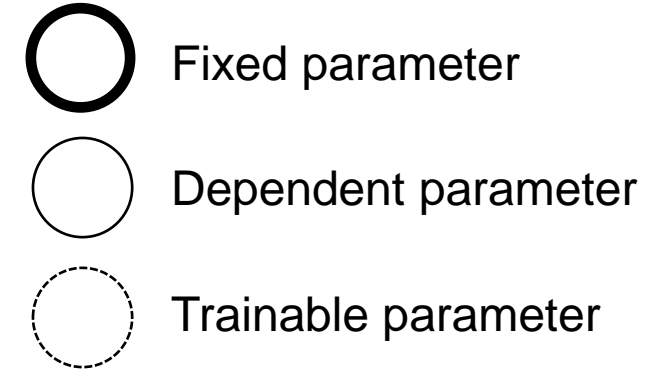
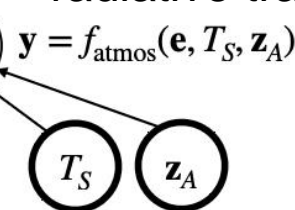
0.6 billion observations
4.9 billion inputs
91 million trainable state parameters
80 trainable model parameters
4 additional loss terms
Tensorflow/Keras training

Bayesian network representation of the “sea ice” model – which is then implemented and solved using Tensorflow/Keras

AMSR2 observations



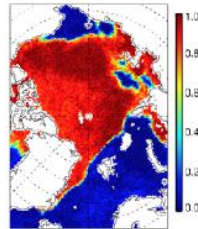
Known atmosphere radiative transfer



Surface emissivity

$e = C_{\text{ice}} e_{\text{ice}} + (1 - C_{\text{ice}}) e_{\text{wat}}$

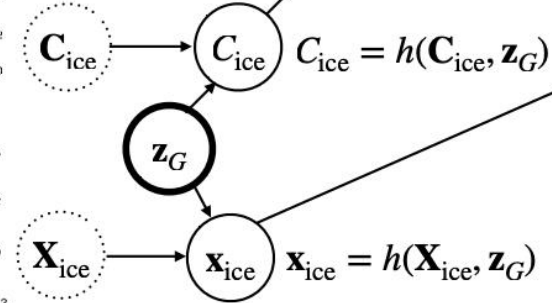
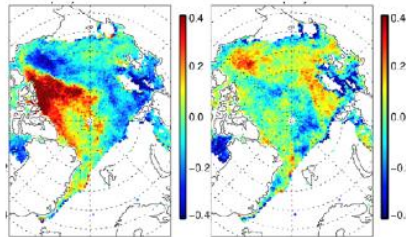
365 day maps of sea ice fraction



Known water surface emissivity



365 day maps of empirical parameters



Empirical neural network for sea ice emissivity

$e_{\text{ice}} = f_{\text{empirical}}(w, x_{\text{ice}}, z_B)$

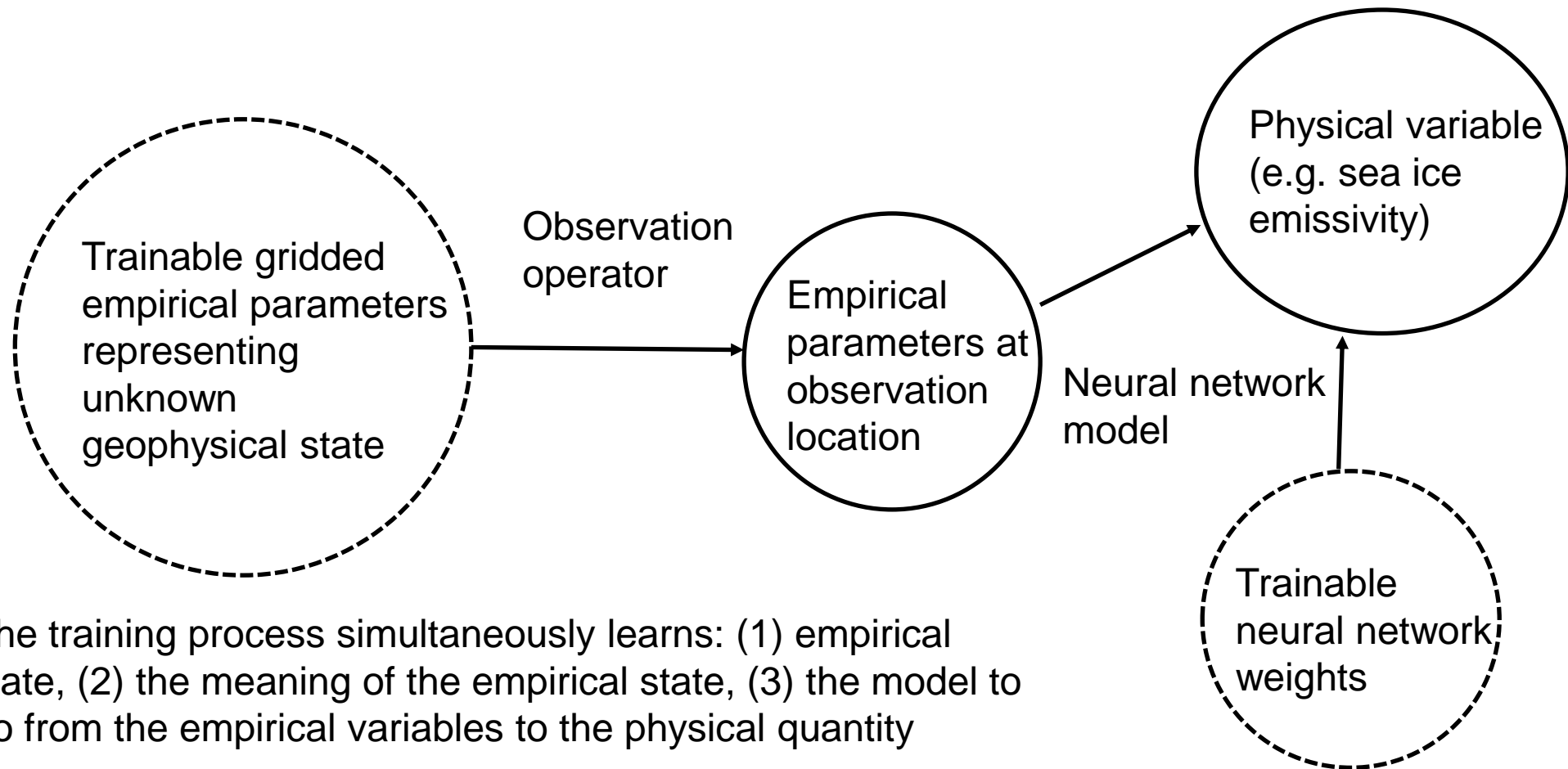


w – trainable weights of NN model for sea ice



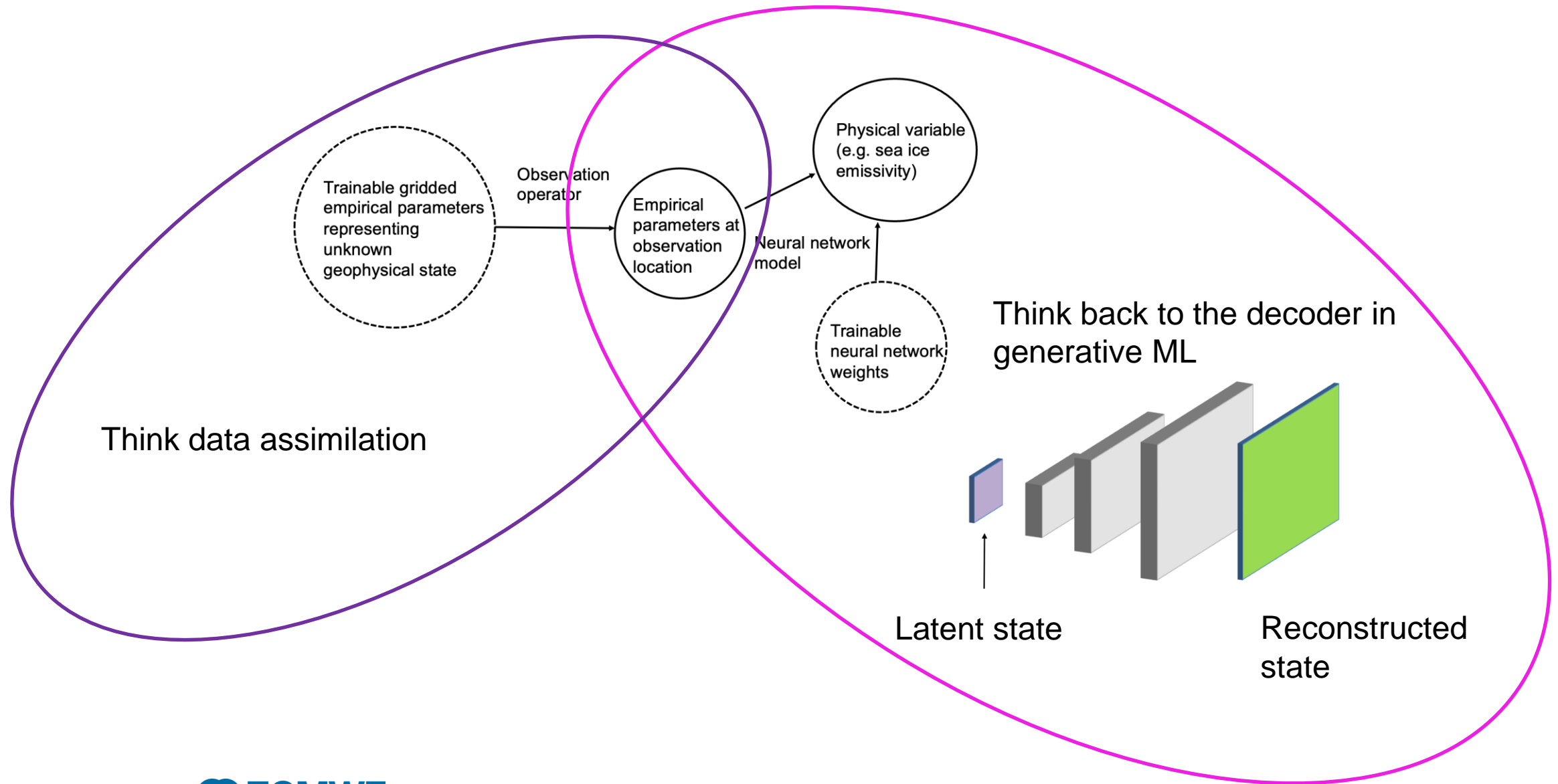
h() Observation operator: map to observation location in time and space

Fundamentals of this “Empirical state” method



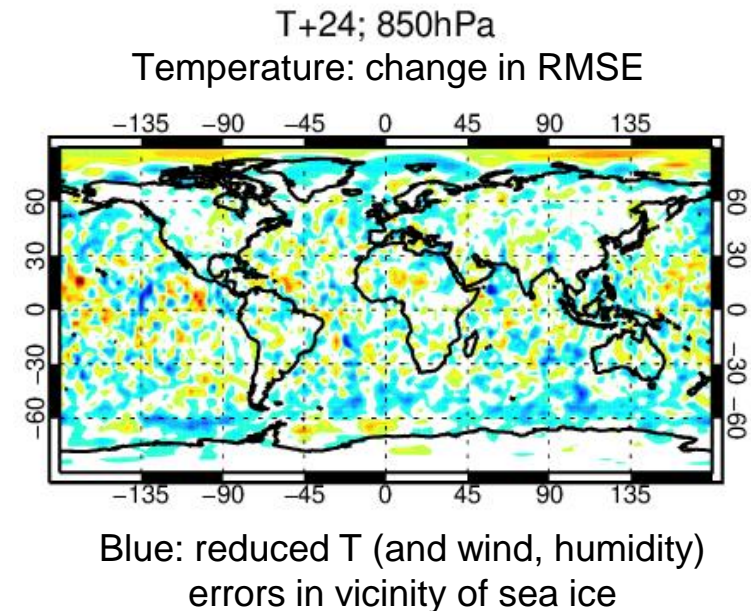
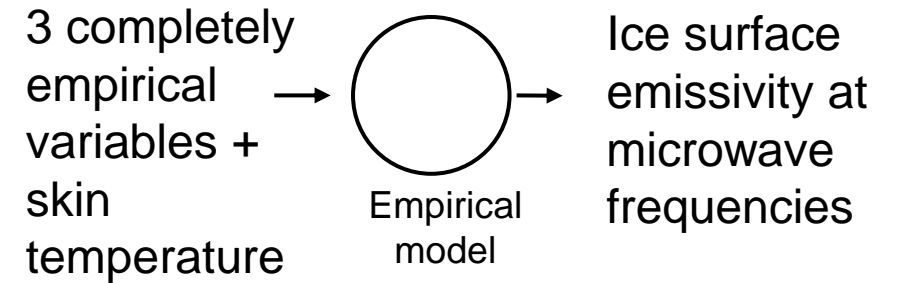
The training process simultaneously learns: (1) empirical state, (2) the meaning of the empirical state, (3) the model to go from the empirical variables to the physical quantity

Fundamentals of this “Empirical state” method



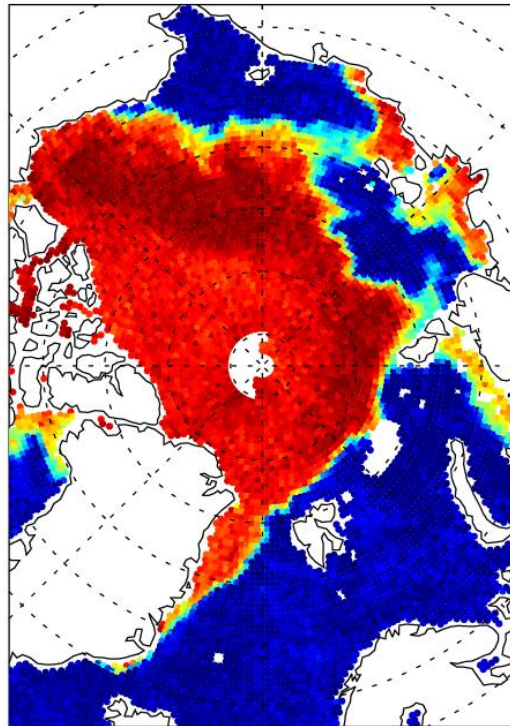
Sea ice surface emissivity model in the IFS

- Surface emissivity model trained offline (previous slide)
- Use this as a fixed model (no further training) within the IFS 4D-Var for assimilating microwave observations over sea ice
- Where do the empirical inputs come from?
 - Retrieve them from the observations as part of 4D-Var (sink variable approach)
- Why?
 - Retrieve high quality sea ice fraction directly within the atmospheric 4D-Var system
 - Use surface-sensitive microwave observations in sea ice areas and in close proximity ocean areas -> significant improvements in Southern ocean forecast skill
- To be implemented operationally in June 2024 as part of IFS cycle 49r1 (hopefully)

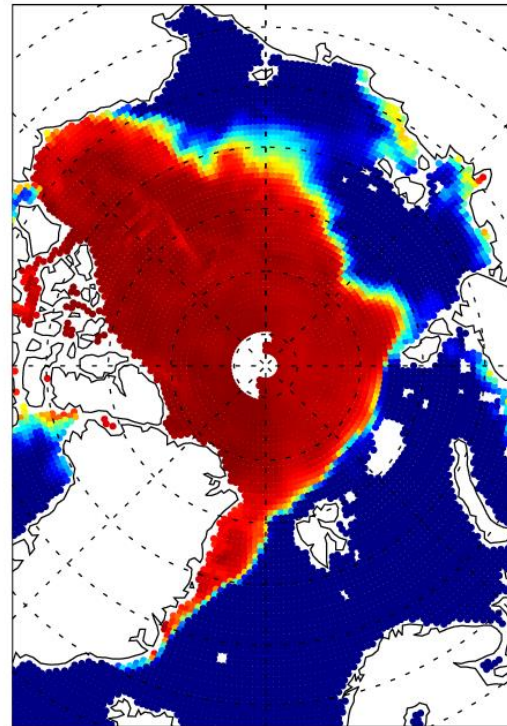


Sea ice fraction retrieval: rapid freezing 2nd Nov 2020

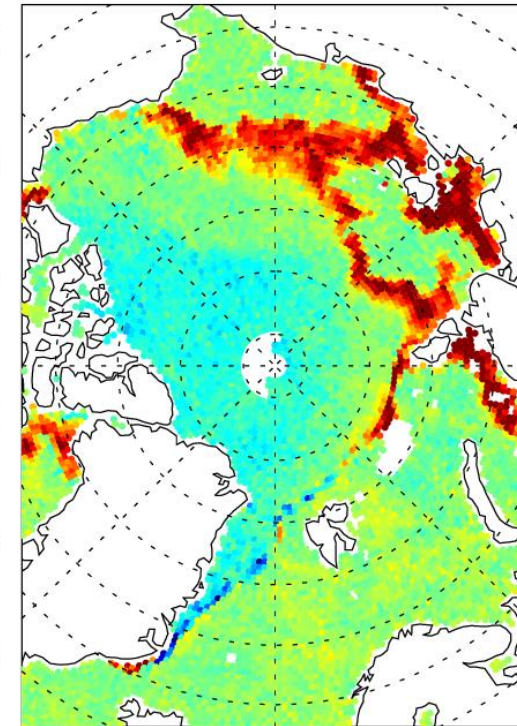
New retrieval from AMSR2



Current IFS (OCEAN5)



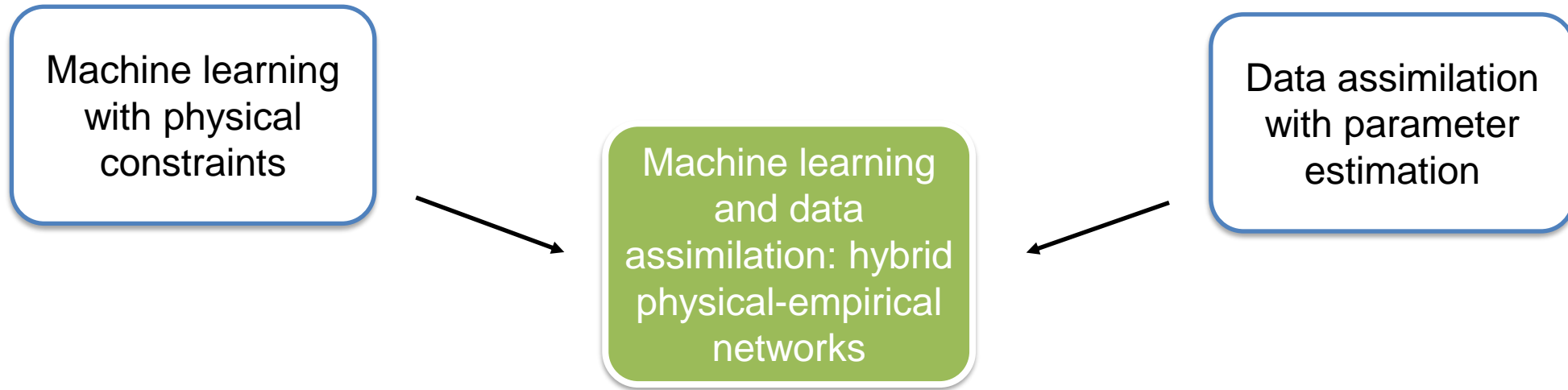
Retrieved – current IFS



Difference
in sea ice
fraction

IFS estimate is delayed by up to about 48 hours due to a very long processing chain

Summary: generating new empirical models using ML and DA



- Typical machine learning and variational data assimilation are similar implementations of Bayes' theorem
- Including known physics into a trainable network is a way of adding prior information in a Bayesian sense
- Existing data assimilation approaches can be very helpful in machine learning:
 - Physically-based loss functions
 - Physically-based observation (label) and background (feature) errors
 - Observation operators to map from grid to irregular and transformed observation space (e.g. satellite radiances)
- Data assimilation frameworks (e.g. weather forecasting) are evolving to be able to train and update empirical models (e.g. neural networks) as part of routine data assimilation activities
 - E.g. model error correction: don't throw away the physical model – improve it!